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A RESERVOIR SIMULATOR.

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COMPOSITIONAL FLOW IN POROUS MEDIA:
A RESERVOIR SIMULATOR

A DISSERTATION
SUBMITTED TO THE GRADUATE FACULTY
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degree of
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FORREST F. CRAIG, III
Norman, Oklahoma
1976

COMPOSITIONAL FLOW IN POROUS MEDIA:

A RESERVOIR SIMULATOR

APPROVED BY:

Harry Crichton

K E Stirling

D E Menzie

Martin E. Chenevert

James Hristov

DISSERTATION COMMITTEE

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COMPOSITIONAL FLOW IN POROUS MEDIA:

A RESERVOIR SIMULATOR

INTRODUCTION

. . . [The phase behavior portion] of the problem will be treated by making the conventional assumption that "gas is gas", although this must be recognized as a basic weakness.
(Muskat, [1], p. 381)

Muskat was only one of the many early investigators to recognize that the phase behavior aspects of the reservoir engineering analysis have traditionally been greatly oversimplified. Advances over the past decade or so in computing machinery and numerical techniques now present a means of treating the general reservoir problem, and specifically the hydrocarbon phase behavior problem, in a more rigorous manner.

This investigation attempts to formulate a general phase behavior algorithm consistent with the fundamentals of phase behavior which can be easily modified to describe observed fluid and reservoir behavior. This algorithm will be incorporated in a numerical reservoir simulation model. The main emphasis of this work will be to produce an efficient, flexible, and reasonably useful reservoir simulation package, concentrating on the development of the phase behavior algorithms.

CHAPTER I

HISTORY OF RESERVOIR SIMULATION

The engineer is constantly attempting to describe physical systems in mathematical terms. This effort to simulate the behavior of physical systems begins by making a great many assumptions to simplify the problem to a level which can be easily handled. As expertise in a given area increases, fewer simplifying assumptions are made and the solutions obtained begin to match the physical problem more closely. At each stage of improvement in the model, the engineer who uses it must be aware of the assumptions involved in order to fully understand the results obtained.

The same method of development has occurred in reservoir simulation. The initial effort to model a reservoir system was the zero-dimension material balance method. This procedure was based on a great many assumptions but provided the engineer with an indication of the expected behavior of a reservoir system. The natural next step in the advancement of simulation was the expansion of the zero-dimensional model to a one-dimensional scheme. This procedure has the advantages of fewer assumptions, greater flexibility, and as a result, greater applications and efficiency. In order to

obtain these advantages, the amount of computation is increased and there are a great many additional variables which must be included to describe the physical behavior in each cell of the system.

With the increasing availability of computers and their greater storage and faster computation speeds, the two-dimensional system was used to describe reservoir systems even more accurately. Although three-dimensional systems are now available, the most popular simulator is the two-dimensional procedure because a well-organized two-dimensional simulator can be used to approximate three-dimensional reservoir behavior. This results in a savings in execution time and storage requirements as a result of fewer cells, which is desired from an economic viewpoint. Two-dimensional models can be run on smaller computer systems and at a lower price than a three-dimensional model of the same system. The additional accuracy of a three-dimensional model is seldom justified due to the inaccuracies of the data input. No matter how well a model obeys the equations which describe real behavior, it is only as accurate as the information which is available on the reservoir properties.

Along with the advent of simulators which describe reservoir systems in multi-dimensional form, an effort was made to duplicate the behavior of the fluids present. The traditional approach (often called the black-oil method) was to view the fluid as several independent phases which had no interaction. As expertise increased in fluid behavior and

mathematical techniques of analysis, efforts were made to incorporate more accuracy into simulators. This was done in many ways, but the most popular was to use a table of lookup or polynomial curve fit of the fluid properties which required a minimal amount of additional storage. This resulted in a more realistic model, but this approach to the fluid properties assumed that they were functions of only pressure in an isothermal system, that interphase mass transfer did not occur, and that the phase composition did not change. The next advance was to use a compositional approach in which the fluid properties are described as functions of pressure, temperature, and composition of the fluids. A basic assumption involved in the compositional approach is that the water phase exists only as a liquid, while the hydrocarbon portion of the fluid can exist in either a gas or liquid phase. This approach requires the storage of not only the fluid properties for each cell, but also the vapor and liquid phase compositions (one variable for each component in each cell). The determination of the phase compositions for each cell requires increased computer time compared with the black-oil approach. Again, the model is only as good as the input data and the accuracy of the equations used.

The primary effort in this study is to develop a two-dimensional, compositional reservoir simulation package. Special attention will be paid to the fluid properties portion, particularly to the flash determination of the phase compositions. The use of compatible fluid property correlations for

the liquid and vapor phases is essential in the compositional approach. The correlations must produce a continuous function, especially at the critical point of the hydrocarbon mixture where the vapor and liquid properties are required to become indistinguishable. Minimization of computer storage and execution time is also a concern in order to provide an economical simulation package. Because compositional packages are, by nature, lengthy projects which require many man-years to optimize, this study will lay the foundation for a long term program. All of the components needed in a compositional simulator will be developed, any problem areas pinpointed, and recommendations will be made on a possible plan of research to improve these areas.

CHAPTER II

MECHANICS OF COMPOSITIONAL FLOW

A compositional model is one in which the phase behavior of the fluids in the reservoir is taken into account. It differs from a traditional black-oil model in that inter-phase mass transfer is considered and the individual components are treated, along with pressures and phase saturation, as separate variables. In order to understand the development and advantages of a compositional reservoir model, one must first understand the mechanics of compositional flow.

Three-Phase Flow in Porous Media

Nearly all naturally occurring petroleum reservoirs consist of water-wet rock systems. These reservoirs, sometimes called hydrophilic reservoirs, exhibit the following distribution when a water-oil-gas system is present:

Water fills the smallest pores completely and wets the surface of all of the rock grains.

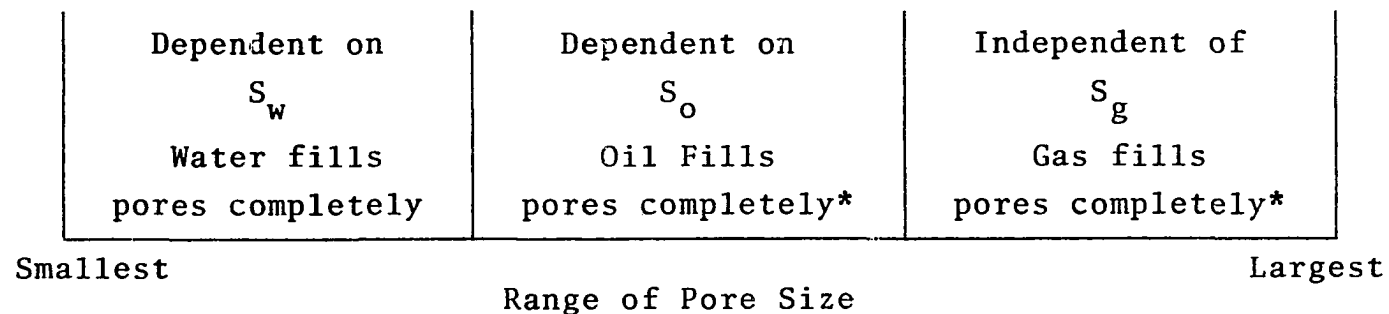
Oil fills a range of pores beginning with those which just exceed the maximum size completely filled with water. The amount of oil in the system determines the largest pore which is filled by the oil phase.

Gas fills the remainder of the pores, from those which just exceed the maximum size completely filled with oil to the largest pores present in the system. Because of the highly compressible nature of gases, this phase will expand to fill all of the pores not occupied by one of the other phases.

This behavior is shown diagrammatically in Figure 1. As would be expected, the pore sizes in naturally occurring rock are randomly distributed throughout the system. Macroscopically, the three phases appear to be well mixed because of the random pore distribution. There is ample opportunity under flow conditions for the phases to contact each other and for phase changes to occur.

Classification of Reservoir Fluids

Each hydrocarbon system has its own phase diagram. A typical phase diagram, which depends only on the fluid composition, is presented in Figure 2. The critical point is that point where the liquid and vapor phases become indistinguishable. The composition, density, viscosity, and all other properties of one phase become identical to the corresponding property of the other phase at the critical point. The cricondentherm is defined as the maximum temperature at which a two-phase region can exist for a given fluid. The two-phase region is that area of the pressure-temperature phase diagram which is between the bubble point and dew point curves. This is the region where the reservoir fluid exists in equilibrium as both a gas and a liquid. Outside this



∞

*except for surface of rock grains which are wet by water in hydrophilic systems.

Figure 1
Fluid Distribution in Pores

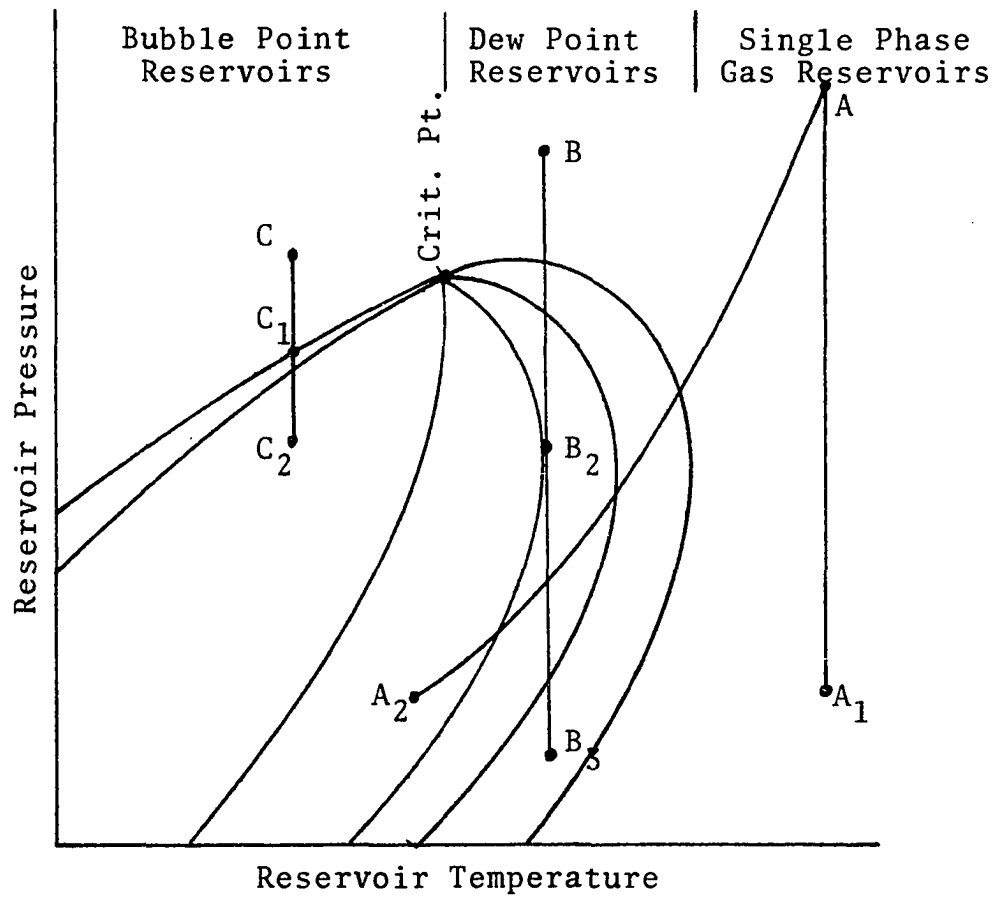


Figure 2

Pressure-Temperature Phase Diagram for
a Multicomponent Hydrocarbon System

region, the fluid exists only in one phase (liquid or gas). Reservoirs and the fluids they contain are classified based on the location on the phase diagram of the point which represents the initial temperature and pressure of the hydrocarbon mixture with respect to the critical point, the cricondentherm, and the two-phase region.

For a reservoir fluid which exists at the initial pressure and temperature conditions of point A on the phase diagram, we observe fluid behavior which follows the path from A to A_1 as the reservoir is depleted isothermally. Because the temperature of the reservoir exceeds the cricondentherm, the fluid in the reservoir will remain in a single (vapor) phase. This type of reservoir is called a single-phase gas system. During production, the fluid temperature and pressure decrease as the hydrocarbon mixture moves toward the surface. If the path of production enters the two-phase region, as in this case (path A - A_2), a liquid phase will condense out of the vapor and be produced from surface separators, although the fluid in the reservoir will continue to be single phase.

If the reservoir temperature lies between the critical temperature and the cricondentherm of the given hydrocarbon system and in the one-phase region, isothermal depletion of this gas system follows the path B - B_3 . This system is called a retrograde gas-condensate or dew-point reservoir. As the reservoir pressure decreases, the phase path intersects the dew point curve. At this point (B_1) liquid begins

to form and the liquid volume present increases to a maximum at point B_2 . From this point to B_3 , the amount of liquid present decreases until abandonment pressure. Of course, if the abandonment pressure causes the path to cross the lower portion of the dew point curve, the reservoir fluid will again be a single (vapor) phase. It should be pointed out that the liquid phase which condenses forms on the pore surfaces of the rock and has a very low mobility. Thus, the composition of the reservoir fluid is constantly changing as the light hydrocarbon components are produced in the vapor phase while the heavy components condense out in a mostly unrecoverable liquid phase. This means the pressure-temperature phase diagram is constantly shifting downward and to the right (as the reservoir fluid composition changes), which further aggravates the retrograde liquid loss. If the reservoir pressure is maintained by natural water influx or gas cycling, this retrograde loss is reduced.

A bubble-point reservoir is characterized by an initial temperature less than the system critical temperature and an initial pressure greater than the bubble point pressure. Because of the low compressibility of liquids, the pressure decreases rapidly along the path $C - C_1$, as the reservoir liquid is produced. At point C_1 , a vapor phase begins to form. Because this gas phase has a much higher mobility than the liquid phase, the gas-oil ratio for the produced fluid increases rapidly. When an active water drive is present, the reservoir pressure is at least partially

maintained. Because the reservoir pressure remains above the bubble pressure for a longer period of time, the single phase liquid flow into the well is maintained longer, so the oil recovery is higher. As in a retrograde reservoir, the vaporization of the light components and the high gas-oil ratio causes the composition of the reservoir fluid to shift continually. The phase diagram shifts to the right and downward which accentuates the decrease in the liquid recovery. In those cases where the shift is serious, the bubble-point reservoir is also called a volatile oil reservoir.

The fourth and final type of reservoir is the two-phase system. This type of reservoir is one with an initial temperature and pressure which falls inside the two-phase envelope of the pressure-temperature phase diagram. The gas cap phase produces as a retrograde or single-phase reservoir, while the liquid phase produces as a bubble-point reservoir. Each phase produces as a separate type of fluid because the vapor and liquid each have different compositions and thus different phase diagrams.

The four types of reservoir fluids are presented in Figure 3. The single-phase gas type is indicated by a reservoir temperature greater than the cricondenthem of the system, while a gas condensate reservoir is present when the reservoir temperature is less than the cricondenthem but greater than the critical temperature. The volatile oil and dark oil types of systems are different sub-types of bubble-point systems (a reservoir temperature less than the system critical

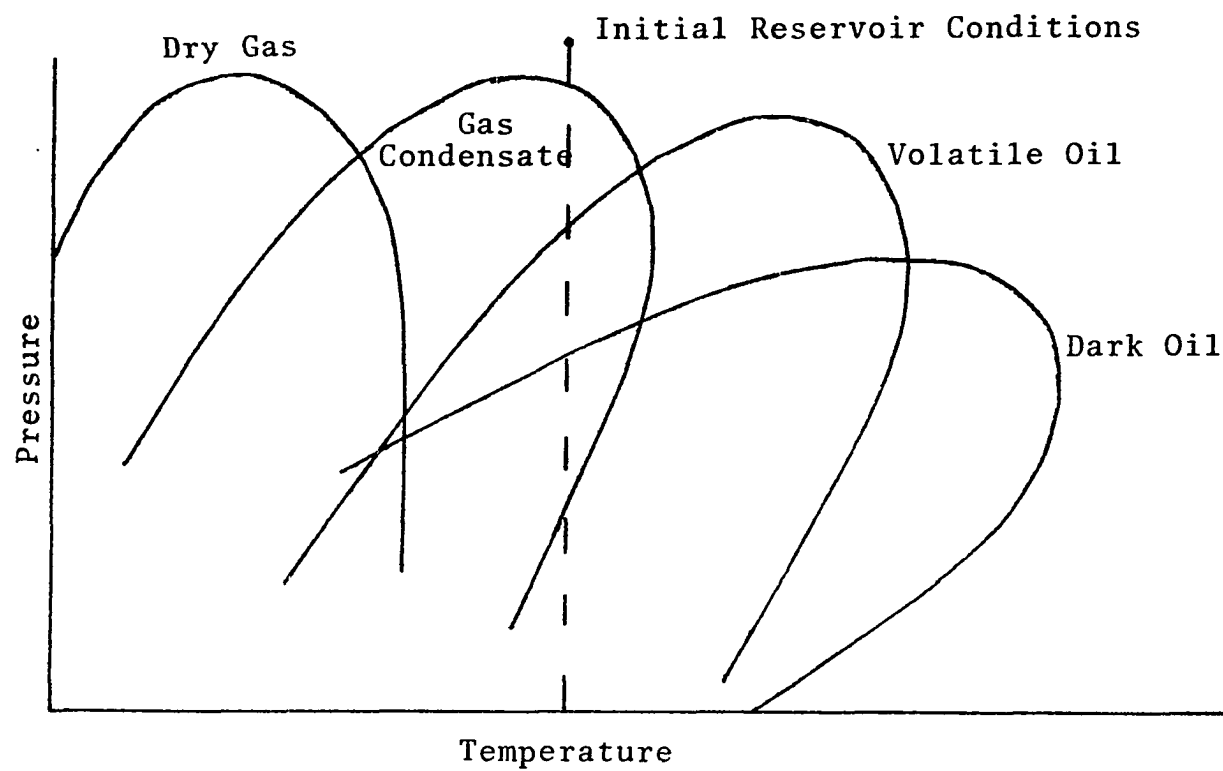


Figure 3

Types of Reservoir Systems

temperature) and are differentiated by the amount of shift of the composition, or phase diagram, which occurs during depletion. These four classifications apply only to reservoir systems which are initially in equilibrium and remain in equilibrium throughout the depletion process. This assumption of equilibrium at all times is a basic assumption used in all reservoir work. Typical compositions of each fluid type are:

	<u>Methane (mol %)</u>	<u>Intermediates (mol %)</u>	<u>Heptanes+ (mol %)</u>
Dark Oil	30	35	35
Volatile Oil	55	30	15
Gas Condensate	70	22	8
Dry Gas	90	9	1

Because of the serious shift of the volatile oil and retrograde gas-condensate phase diagrams during depletion, the traditional black oil simulator is not sufficiently accurate to provide good performance prediction. In these cases, and others where changes in the composition of the reservoir fluid complicate performance calculations, the compositional model is the best approach to prediction.

CHAPTER III

FLUID PROPERTIES

The system fluid properties are of vital importance in a reservoir simulation model and it is essential that these properties be considered not only as functions of the system temperature and pressure, but also as functions of the system composition. Many published techniques are available for predicting volumes and viscosities of hydrocarbon mixtures based on phase composition data. From these, the most widely used methods have been selected in order to ensure that the method chosen is valid over a broad range of applications. Correlations are taken directly from the literature without modification. The most direct, non-iterative techniques are employed in all cases.

Flash Calculation

One of the most important components of a compositional reservoir simulator is the flash calculation. This is the method by which one can compute the compositions and relative amounts of the vapor and liquid phases of a given hydrocarbon mixture if one knows the overall composition of the mixture and the required equilibrium constants.

This procedure involves a simple trial-and-error material balance on a unit molal mass of the hydrocarbon mixture.

The equilibrium constant is defined as

$$K_i = \frac{y_i}{x_i} \quad (3-1)$$

where x_i and y_i are the mole fraction of each component in the liquid and vapor phases, respectively. The definition of mole fraction provides two more equations.

$$\sum x_i = 1.0 \quad (3-2)$$

$$\sum y_i = 1.0 \quad (3-3)$$

We also know, because there is no chemical reaction, that a molal material balance on our system must be satisfied such that the sum of the number of moles in the liquid and vapor phases must equal the total number of moles in the system, which we will call unity for convenience.

$$L + V = 1.0 \quad (3-4)$$

We can also express the overall mole fraction of a particular component in terms of the mole fractions of this component in each phase and the number of moles in each phase.

$$z_i = x_i L + y_i V \quad (3-5)$$

We can then use the definition of the equilibrium constant to eliminate the vapor mole fraction term or the liquid mole fraction term.

$$z_i = x_i (L + K_i V) \quad (3-6)$$

$$z_i = y_i (L/K_i + V) \quad (3-7)$$

Solving for each phase mole fraction and realizing that the mole fractions in each phase must sum to unity and thus the difference of the two sums must be zero, the above equations become

$$\sum_{i=1}^n \frac{z_i}{(L + K_i V)} - \sum_{i=1}^n \frac{z_i K_i}{(L + K_i V)} = 0.0 \quad (3-8)$$

Combining the terms and using equation (3-4) to eliminate the term for the number of moles of vapor, we obtain the final form of the flash equation.

$$\sum_{i=1}^n \frac{z_i (1 - K_i)}{L(1 - K_i) + K_i} = 0.0 = f(L) \quad (3-9)$$

The only unknown in this equation is the number of moles per total moles of the mixture that are in the liquid phase. The Newton-Raphson iteration technique is employed to determine the solution for the liquid split. This method is described by

$$L_{k+1} = L_k - \frac{f(L_k)}{f'(L_k)} \quad (3-10)$$

where k is the iteration counter and L is the mole fraction in the liquid phase. The solution for the liquid phase mole fraction is that value of L which causes $f(L)$ (equation 3-9) to equal zero.

Fortunately, the derivative of the function, which is required for the Newton-Raphson technique, is easily obtained as a direct analytical expression.

$$f'(L) = - \sum_{i=1}^n \frac{z_i (1 - K_i)^2}{[L(1 - K_i) + K_i]^2} \quad (3-11)$$

Studying the above equations reveals some information which will eliminate several worries during the solution of the problem. Obvious difficulties are encountered if the denominator of any of the terms of the function or its derivative become zero, making the value of the function undefined. Thus a singularity exists for each component when

$$L(1 - K_i) + K_i = 0.0 \quad (3-12)$$

The value of L which produces this singularity is

$$L = - \frac{K_i}{(1 - K_i)} \quad (3-13)$$

Because the value of the equilibrium constant, K_i , is always, by definition, larger than zero, the values of L_k at the singularity points are

$$\begin{aligned} \text{for } 0 < K_i \leq 1, \quad L_k &< 0.0 \\ \text{for } 1 < K_i, \quad L_k &> 1.0 \end{aligned}$$

In the interval of physical significance ($0.0 \leq L_k \leq 1.0$), the function is well-behaved.

Noting that, by virtue of the squared terms and the non-negative mole fraction variable, the derivative function is always negative, the Newton-Raphson equation becomes

$$L_{k+1} = L_k + \frac{\sum_{i=1}^n \frac{z_i (1 - K_i)}{[L_k (1 - K_i) + K_i]}}{\sum_{i=1}^n \frac{z_i (1 - K_i)^2}{[L_k (1 - K_i) + K_i]^2}} \quad (3-14)$$

which is solved iteratively over the interval of $0.0 \leq L_k \leq 1.0$.

To determine whether a flash calculation is required, the function is evaluated at $L_k = 0.0$ and $L_k = 1.0$.

$$f(0) = \sum_{i=1}^n \frac{z_i(1 - K_i)}{K_i} \quad (3-15)$$

$$f(1) = \sum_{i=1}^n z_i(1 - K_i) \quad (3-16)$$

By examining the values of these two functions and realizing that the function is always decreasing over the range of significance (i.e., the derivative is always negative), we can determine whether the system is two-phase, entirely liquid, or entirely gas. When $f(0)$ is less than zero, the system is all gas. When $f(1)$ is greater than zero, the system is all liquid. Otherwise, the system is two-phase and the flash calculation must be performed.

A large number of flash calculations are required during a simulator run. Thus, the faster the rate of convergence, the more efficient the simulator will be. For this reason, several different methods of obtaining an accurate initial estimate for the mole fraction of the liquid phase are tested, with the aim of obtaining a method which yields a rapid rate of convergence. Three methods of determining an initial guess for L_0 are tested: $L_0 = 0.5$; linear interpolation between $f(0)$ and $f(1)$; and Lagrangian interpolation with $f(0)$, $f(0.5)$ and $f(1)$. As can be seen in Table 1, the

Table 1

Rate of Convergence for Three Methods of Obtaining
Initial Guess for Flash Calculation

Liquid Split Range	Samples In Range	Iterations Required for Solution*			Best Method
		1	2	3	
0.00 - 0.05	5	31	29	28	3
0.05 - 0.10	10	109	95	104	2
0.10 - 0.15	13	140	143	79	3
0.15 - 0.20	16	137	116	76	3
0.20 - 0.25	10	58	54	38	3
0.25 - 0.30	7	33	31	27	3
0.30 - 0.35	4	17	16	13	3
0.35 - 0.40	6	27	27	19	3
0.40 - 0.45	6	20	28	16	3
0.45 - 0.50	5	12	21	11	3
0.50 - 0.55	2	6	8	4	3
0.55 - 0.60	2	9	11	6	3
0.60 - 0.65	3	11	11	7	3
0.65 - 0.70	3	12	11	7	3
0.70 - 0.75	2	8	6	4	3
0.75 - 0.80	4	16	12	10	3
0.80 - 0.85	3	12	9	6	3
0.85 - 0.90	2	8	6	4	3
0.90 - 0.95	0	0	0	0	-
0.95 - 1.00	2	8	4	3	3
Totals	106	669	638	462	

*Method 1 - Initial Guess = 0.50

Method 2 - Linear Interpolation Between $f(0) + f(1)$

Method 3 - Lagrangian Interpolation Between $f(0)$, $f(.5)$,
+ $f(1)$

initial guess using Lagrangian interpolation is found to be superior to the others.

For 106 samples, randomly scattered throughout the range possible for liquid split values, an average of 6.3 flash iterations are required to obtain a solution for each sample when the initial guess for the liquid split is 0.5 (the middle of the possible range for L). When using linear interpolation between $f(0)$ and $f(1)$ to obtain an initial guess for the value of L which satisfies the relation $f(L) = 0.0$, the average number of flash iterations required to obtain a solution is 6.0 for each sample. This is only a slight increase in the accuracy of the initial guess and is obtained at an overall increase in the amount of computations required. It is found that the overall efficiency of the flash routine is increased by using Lagrangian interpolation between $f(0)$, $f(.5)$ and $f(1)$. An average of only 4.4 flash iterations are required for solution.

The determination of the initial guess using Lagrangian interpolation requires approximately the same number of calculations as a single flash iteration using the Newton-Raphson procedure. Many of the calculations required for the Lagrangian method are necessary for the test, discussed previously, to determine if the system is two-phase, resulting in the addition of very little computation in order to use the Lagrangian procedure. Thus, if the use of this fairly complex method of obtaining an initial guess increases the rate of convergence enough to eliminate only one

iteration, a net increase in efficiency is obtained.

Thus, the initial guess for L_o is defined as

$$\begin{aligned}
 L_o = & \frac{f(L) - f(.5)}{f(0) - f(.5)} * \frac{f(L) - f(1)}{f(0) - f(1)} * 0 \\
 & + \frac{f(L) - f(0)}{f(.5) - f(0)} * \frac{f(L) - f(1)}{f(.5) - f(1)} * .5 \\
 & + \frac{f(L) - f(.5)}{f(1) - f(.5)} * \frac{f(L) - f(0)}{f(1) - f(0)} * 1.0
 \end{aligned} \tag{3-17}$$

which, realizing that at the value of L which is the desired solution, $f(L)$ is zero, the above equation becomes

$$\begin{aligned}
 L_o = & \frac{f(0)}{f(.5) - f(0)} * \frac{f(1)}{f(.5) - f(1)} * .5 \\
 & + \frac{f(.5)}{f(1) - f(.5)} * \frac{f(0)}{f(1) - f(0)} * 1.0
 \end{aligned} \tag{3-18}$$

This method is only used during the first flash calculation or for cells which later produce L values within 0.05 units of either boundary of the permissible range. Because only a slight change in the L value is expected for non-producing cells in the reservoir simulator, on each successive use of the flash calculation the most recent L value for that cell will be used as an initial guess.

If the Newton-Raphson technique produces a value of L_k outside the permissible range, the value of L_k is reset to zero or one, whichever is nearer the errant value of L_k .

Equilibrium K-Value Determination

The flash calculation procedure outlined previously requires values for the equilibrium constants of each

component as a function of system temperature, pressure, and convergence pressure (which is a measure of the fluid composition). The most commonly used correlations for equilibrium constants are the Natural Gas Processors Suppliers Association (NGPSA) K-value charts. These log-log charts, based on experimental data tabulated in 1947 by G. G. Brown at the University of Michigan, are available for fourteen hydrocarbon components plus nitrogen and hydrogen sulfide and at seven convergence pressures ranging from 800 psia to 10,000 psia.

The NGPSA charts and the theory of corresponding states are used as the basis of an algorithm to estimate the equilibrium ratios required in this investigation. The Canfield [2] equation is used as a basis for the study. It is of the form:

$$K = \frac{1}{P_R} \exp \left[\left(10.7016 - \ln P_{\text{conv}} - \frac{4.4316}{T_R} - \frac{.1968}{T_R^3} \right) \times (6.3816 - 29.0020 Z_C + 35.3443 Z_C^2) (1. - P_R)^{.33/T_R} \right] \quad (3-19)$$

Before development of the correlation, it would be appropriate to discuss constraints placed on K-value behavior by a viable reservoir simulation model. Fussell and Yarbrough [3] have pointed out that, primarily because the derivative of the K-values with respect to both pressure and composition (expressed as convergence pressure) is used implicitly in the numerical solution to the model's basic

diffusivity equations, the simulator's results are very sensitive to the smoothness of the equilibrium ratio relationships. A further constraint, of course, is the fact that by definition the equilibrium ratio must equal 1.0 when the system pressure is equal to the convergence pressure.

Smith and Van Ness [4] indicate that for an ideal liquid solution and an ideal gas phase, the equilibrium ratio is simply and exactly the ratio of the component vapor pressure to the total system pressure. Hougen, Watson, and Ragatz [5] give an equation for the reduced component vapor pressure,

$$\log_{10} P_{RS} = \frac{-A(1 - T_R)}{T_R} - 10^{-8.68(T_R - B)^2} \quad (3-20)$$

where

$$A = 16.25 - 73.85 Z_c + 90.00 Z_c^2 \quad (3-21)$$

$$B = 1.80 - 6.20 Z_c \quad (3-22)$$

Using this reduced component vapor pressure in the equilibrium K-value definition, we obtain

$$K_i = \frac{P_{RS}}{P_R} \quad (3-23)$$

The easiest correction of this equation to allow for real systems is to multiply the pressure ratio by a correction factor. Several such correction factors have been proposed in the literature, such as that set forth by Canfield [2] (who ignores the reduced component vapor pressure):

$$C = \exp \left[\left(10.7016 - \ln P_{\text{conv}} - \frac{4.4316}{T_R} - \frac{.1968}{T_R^3} \right) \times (6.3816 - 29.0020 Z_c + 35.3443 Z_c^2) (1 - P_R)^{.33/T_R} \right] \quad (3-24)$$

or that suggested by Hougen, Watson, and Ragatz [5]:

$$C = \exp \left[\frac{Z_c}{T_R} (.25 + .132 T_R) (P_R - P_{RS}) \right] \quad (3-25)$$

Because the forms of the two equations are similar and the Hougen, Watson, and Ragatz [5] equation is consistent in terms of the use of a reduced component vapor pressure, it is chosen as a new basis for an improved K-value correlation.

The obvious error of the Hougen, et al. [5] equation is its failure to converge to a value of 1.0 when the system pressure is equal to the convergence pressure of the system. This is corrected by including a term so that the improved equation becomes

$$K_i = \left\{ \frac{P_{RS}}{P_R} \exp \left[\frac{Z_c}{T_R} (.25 + .132 T_R) (P_R - P_{RS}) \right] \right\}^\alpha \quad (3-26)$$

where

$$\alpha = (1 - P/P_{\text{conv}})^\beta \quad (3-27)$$

It is found that the value of β is a function of the reciprocal of the reduced temperature, which agrees well with the similar term in the corresponding states K-value algorithm developed by Canfield. Optimization procedures, undertaken to determine the value of β which yields the best

results, indicate that β is also a function of the convergence pressure. The modified equation, after optimization, becomes

$$K_i = \left\{ \frac{P_{RS}}{P_R} \exp \left[\frac{Z_c}{T_R} (.25 + .132 T_R) (P_R - P_{RS}) \right] \right\}^\alpha \quad (3-28)$$

where

$$\alpha = (1 - P/P_{conv})^\beta \quad (3-29)$$

$$\beta = \frac{1}{T_R} [(1.4 * 10^{-4}) P_{conv} + .08] \quad (3-30)$$

This equation is developed using 360 data points, five pure components (methane, ethane, propane, n-butane, n-pentane), three convergence pressures (1000, 2000, and 5000 psia), six pressures, and four temperatures for each component, and produces an overall average absolute error of 19.3% compared with 39.6% for the Hougen, et al. [5] equation and 37.5% for the Canfield [2] equation. Further attempts to improve this algorithm produce a highly complicated equation with only a slight improvement in accuracy.

This correlation, although superior to the Canfield [2] or Hougen, et al. [5] corresponding states algorithms, fails to provide the accuracy or smoothness which Fussell and Yarborough [3] point out is necessary for use in a compositional simulator. Several factors involved in the development of this correlation may be at fault.

The first and most obvious is the possibility that the theory of corresponding states is not valid for use in predicting equilibrium K-values. More likely, the

corresponding states correlations used as a basis in this investigation contain weaknesses which have not been corrected.

Another potential source of inaccuracies is the use of Natural Gas Processors Suppliers Association equilibrium K-value charts rather than real data as a source of values upon which this correlation was based. The smoothing, interpolation, and extrapolation involved in the NGPSA charts brings some of the accuracies into question when applied to real systems. K-values for pure component systems, in addition, cannot be accurately used to predict the vapor-liquid split of complex mixtures.

Further work on improving the K-value procedure will undoubtedly result in an improvement of the compositional simulation package.

Convergence Pressure

The equilibrium K-value algorithm discussed requires a system convergence pressure value. Two promising techniques for evaluating the convergence pressure are available in the literature. The approach used by Simon and Yarborough [6] is highly empirical but is based on data from 14 reservoir systems. Etter and Kay [7] approach the problem by attempting to combine the pseudo-critical pressure contribution of each component and what the authors call an excess critical pressure term for each component.

MacDonald [8] investigated both methods of obtaining the system convergence pressure and compared the accuracy

of each. He indicates that for natural gases, multi-component mixtures with no C_{7+} , and ternary mixtures, the Etter-Kay [7] procedure produced results with an average percent error of 6.4, based on 200 examples, compared with 59.7 percent based on 129 samples obtained using the Simon-Yarborough [6] procedure. For reservoir oil systems containing C_{7+} , the Simon-Yarborough [6] procedure is only slightly more accurate (10.1 percent error based on 70 mixtures compared with 11.6 percent based on 75 samples). Because the Etter-Kay [7] method is at least as accurate as the Simon-Yarborough [6] procedure and, in addition, takes the system composition more heavily into account, this procedure was selected to determine the system convergence pressure to be used in the equilibrium K-value correlation.

The Etter-Kay [7] method is very straightforward and defines the convergence pressure, sometimes called the mixture critical pressure, to be

$$P_c = \sum_{i=1}^n Z_i P_{c_i} + \sum_{i=1}^{n-1} \phi_i \quad (3-31)$$

where ϕ_i is the excess critical pressure due to each component and the remainder of the variables are as defined in Appendix A. The first summation is the system pseudo-critical pressure, while the second summation is the system excess critical pressure and includes all but the heaviest component. The excess critical pressure for each component is a function of the weight fraction of each component

$$w_i = \frac{M_i Z_i}{\sum_{j=1}^n Z_j M_j} \quad (3-32)$$

and the average molecular weight of the mixture

$$M_{av} = \sum_{j=1}^n w_j M_j \quad (3-33)$$

If methane is present in the system under study, its excess critical pressure is determined as a special case.

$$\phi_1 = a_1 w_1^{b_1} (M_{av} - M_1) \quad (3-34)$$

The remainder of the component excess critical pressures are determined from the general formula

$$\phi_j = a_j \left[\frac{Z_j}{1 - \sum_{i=1}^{j-1} Z_i} \right]^{b_j} \left[\frac{M_{av} - \sum_{i=1}^{j-1} M_i w_i}{1 - \sum_{i=1}^{j-1} w_i} - M_j \right] \left(1 - \sum_{i=1}^{j-1} Z_i \right) \quad (3-35)$$

where the constants a_j and b_j are defined by Etter and Kay [7] and presented in Table 2. As indicated in the table,

Table 2

Constants for Etter-Kay Convergence Pressure Technique

<u>i</u>	<u>Components</u>	<u>a_j</u>	<u>b_j</u>
1	Methane + Nitrogen	137.	1.073
2	Ethane + Carbon Dioxide	28.6	1.595
3	Propane + Hydrogen Sulfide	13.6	1.225
4	n-Butane + i-Butane	9.24	1.284
i > 4		$9400 M_i^{-1.71}$	$2.000 M_i^{-0.115}$

non-hydrocarbon constituents are included with hydrocarbons of similar molecular weights. Isomers of butane are considered to be the same component, while components containing more than four carbon atoms per molecule have constants defined as functions of the molecular weight of each.

The correlation developed by Etter and Kay [7] is limited to applications to normal paraffin mixtures of low molecular weight. MacDonald [8] has shown that extension of this procedure to heavy hydrocarbon mixtures of high molecular weight is justified if a critical pressure of 6000 psia is used for heptane-plus fractions that may be present.

Liquid Density

Yen and Woods [9] and Guerrero [10] have developed correlations for the liquid volume of a hydrocarbon mixture. The former technique is valid only for pseudo-reduced temperatures less than 1.0, a much smaller range of values than desired, while Guerrero [10] states that his procedure is not valid for reservoir conditions. Kennedy, Bowman, Crownover, and Miesch [11] have developed a very complex correlation which involves several sets of constants and a great deal of calculation. Avasthi and Kennedy [12] present improvements in the Alani and Kennedy [13] method, yet these improvements have been made at the cost of considerable increase in the complexity of the equations used and do not appear to have a significant effect on the accuracy.

The Alani-Kennedy [13] method of determining the liquid volume is selected as the best combination of high

accuracy and ease of computation. This method is based on van der Waal's equation of state which is manipulated to obtain a cubic equation, with constants defined by Alani and Kennedy [13], which can easily be solved directly using procedures available in standard math tables [14]. The authors define mixing rules for a_m and b_m

$$a_m = \sum_{i=1}^n x_i a_i \quad (3-36)$$

$$b_m = \sum_{i=1}^n x_i b_i \quad (3-37)$$

where a_i and b_i are functions of temperature for pure components

$$a_i = K_i \exp[n_i/T] \quad (3-38)$$

$$b_i = m_i T + C_i \quad (3-39)$$

The values of K , n , m , and C are the constants which are defined by Alani and Kennedy [13]. If the mixture contains a heptanes-plus pseudo-component, the authors define a_i and b_i as

$$\begin{aligned} \ln a_{C7+} = & .0038405985 M_{C7+} - .00095638281 \frac{M_{C7+}}{\rho_{C7+}} + \frac{261.80818}{T} \\ & + 7.3104464 * 10^{-6} M_{C7+}^2 + 10.753517 \end{aligned} \quad (3-40)$$

$$\begin{aligned} b_{C7+} = & .03499274 M_{C7+} - 7.2725403 \rho_{C7+} + .0002232395 T \\ & - .016322572 \frac{M_{C7+}}{\rho_{C7+}} + 6.2256545 \end{aligned} \quad (3-41)$$

where M_{C7+} is the molecular weight of the heptanes-plus

fraction, ρ_{C7+} is the density in grams per cubic centimeter of the heptanes-plus fraction at standard conditions (60°F and 14.7 psia), and T is the system temperature in °R. These values are incorporated in van der Waal's equation of state in the form

$$V^3 - \left(\frac{RT}{P} + B_m\right)V^2 + \frac{A_m}{P}V - A_mB_m = 0 \quad (3-42)$$

The liquid volume is defined as the smallest root of this cubic equation.

The authors studied 647 experimental measurements made on 47 reservoir fluid samples in the range of 72°F to 250°F and bubble point to 5000 psig. They found an average deviation of 1.6 percent with a maximum deviation of 4.9 percent.

Constants for three non-hydrocarbon components are obtained by Reamer, Sage, and Lacey [15], Van Itterbeek and Verbeke [16], and Newitt, Pai, Kuloor, and Huggil [17]. The algorithm used includes these parameters plus those developed for hydrocarbons by Alani and Kennedy [13] to ensure its applicability to most typical reservoir fluids encountered. The constants available in the literature are presented in Table 3. It should be pointed out that the constants for methane are valid for the temperature range of 70°F to 300°F, while those for ethane are valid for 100°F to 249°F. Other constants are available for both to 460°F. Because typical reservoirs are less than 250°F, it is not felt to be necessary to include the high temperature constants in the

Table 3
Coefficients Used in the Alani-Kennedy Procedure

Component	K	n	m x 10 ⁴	C
Carbon Dioxide	8,166.	126.	1.818	0.3872
Nitrogen	4,300.	2.293	4.49	0.3853
Hydrogen Sulfide	13,200.	0.	17.9	0.3945
Methane	9,160.6413	61.893223	3.3162472	0.50874303
Ethane	46,709.573	-404.48844	5.1520981	0.52239654
Propane	20,247.757	190.24420	2.1586448	0.90832519
i-Butane	32,204.420	131.63171	3.3862284	1.1013834
n-Butane	33,016.212	146.15445	2.902157	1.1168144
n-Pentane	37,046.234	299.62630	2.1954785	1.4364289
n-Hexane	52,093.006	254.56097	3.6961858	1.5929406
n-Heptane	82,295.457	64.380112	5.2577968	1.7299902
n-Octane	89,185.432	149.39026	5.9897530	1.9310993
n-Nonane	124,062.650	37.917238	6.7299934	2.1519973
n-Decane	146,643.830	26.524103	7.8561789	2.3329874

package. Constants defined for the components other than methane and ethane are not limited by the authors to given temperature ranges.

When components are grouped, a new correlation for the liquid volume must be used, due to the fact that the Alani-Kennedy [13] method can be applied only to pure components. The literature indicates that a reliable, although somewhat complicated, method is the Lee-Edmister modification of the Redlich-Kwong equation of state [18]. This method presents the volume as a function of the composition, critical pressures, critical temperatures, and acentric factors. The cubic equation generated is solved directly, as in the Alani-Kennedy [13] method.

The authors define constants a , b , and c in the following manner.

$$a_m = a_1 - a_2 T + a_3 T^{-1} + a_4 T^{-5} \quad (3-43)$$

$$a_j = (\sum y_i a_{ji}^{1/2})^2 \quad (3-44)$$

$$a_{1i} = \frac{R^2 T_{ci}^2}{P_{ci}} (.25913 - .031314 w_i) \quad (3-45)$$

$$a_{2i} = \frac{R^2 T_{ci}^2}{P_{ci}} (.0249 + .15369 w_i) \quad (3-46)$$

$$a_{3i} = \frac{R^2 T_{ci}^3}{P_{ci}} (.2015 + .21642 w_i) \quad (3-47)$$

$$a_{4i} = \frac{R^2 T_{ci}^7}{P_{ci}} (.042 w_i) \quad (3-48)$$

$$b_m = \sum y_i \frac{RT c_{i1}}{P_{ci}} (.0982) \quad (3-49)$$

$$c_m = c_1 T^{-1/2} + c_2 T^{-2} \quad (3-50)$$

$$c_j = (\sum y_i c_{ji}^{1/3})^3 \quad (3-51)$$

$$c_{1i} = \frac{R^3 T_{ci}^{3.5}}{P_{ci}^2} (.059904) (1 - w_i) \quad (3-52)$$

$$c_{2i} = \frac{R^3 T_{ci}^5}{P_{ci}^2} (.018126 + .091944 w_i) \quad (3-53)$$

where variables are as defined in the Table of Nomenclature in Appendix A. These values are substituted into the Redlich-Kwong equation of state, which is rearranged to the following form

$$V^3 - \frac{RT}{P} V^2 + \left(\frac{a_m}{P} - b_m^2 - \frac{RTb_m}{P} \right) V + \frac{a_m b_m}{P} - \frac{c_m}{P} = 0 \quad (3-54)$$

This cubic equation is solved for the smallest root using the procedure presented in the standard math tables [14]. Nolen [19] found that this procedure is generally unreliable for "a priori" predictions of liquid volumes, but accurate duplication could be achieved by adjusting the critical properties and acentric factors of the heavy hydrocarbon fractions.

The Lee-Edmister [18] method is only used when several components have been grouped into one pseudocomponent. The faster Alani-Kennedy [13] method is used in those

situations where the system consists only of pure components and a heptanes-plus fraction.

The system liquid density is determined by dividing the liquid volume, obtained from one of the above correlations, into the average molecular weight of the liquid system.

Vapor Density

Many methods are available for determining the volume of a hydrocarbon vapor, although most are applicable to pure, ideal components only. Several procedures have been published which are specifically designed for complex hydrocarbon gas mixtures which are encountered in a typical petroleum reservoir. The technique developed by Standing and Katz [20], although relatively accurate, is based on a graphical approach and is not readily adaptable to systems with composition other than those cited by the authors. Kay [21] presents another graphical approach to the determination of the vapor volume. This method is not easily modified for use in a computer model.

The method selected to determine the system vapor volume was that set forth by Sarem [22], which is a curve fit of the Standing and Katz [20] compressibility factor chart as a function of the system reduced-pressure and temperature. The procedure involves the calculation of two dummy variables

$$x = \frac{2P_R - 15}{14.8} \quad (3-55)$$

$$y = \frac{2T_R - 4}{1.9} \quad (3-56)$$

The compressibility factor is then obtained from

$$z = \sum_{m=0}^5 \sum_{n=0}^5 A_{mn} P_m(x) P_n(y) \quad (3-57)$$

where A_{mn} is an element from a 6 x 6 matrix of coefficients and P is a selection of six Legendre polynomials of degree zero through five, as defined by Sarem [22]. This compressibility factor is then incorporated into the real gas law to obtain the vapor volume for the given system. The vapor density is determined by dividing the vapor volume into the average molecular weight of the vapor system.

Viscosities

Several published techniques for determining fluid viscosities are discarded because they are valid for ternary mixtures only (Heric [23]), require values determined graphically (Carr, Kobayashi and Burrows [24]), or are not valid for complex mixtures (Dempsey [25], Lee, Starling, Dolan, and Ellington [26]).

The Little-Kennedy [27] correlation proved to be invalid for a chosen test case, although the authors indicate that some work had been done on complex liquid mixtures. The procedure developed by Lohrenz, Bray, and Clark [28] is selected for determining the liquid viscosity. Although the vapor viscosity technique developed by Lee, Gonzalez, and Eakin [29] seems to be rather simple, yet fairly accurate, the Lohrenz, et al. [28] method is also chosen to determine

the vapor viscosity. This is due to the fact that most of the calculations required for the liquid viscosity are also required for the vapor viscosity, greatly reducing the additional work involved. The Lohrenz [28] method is clearly set forth by Reid and Sherwood [30]. The Stiel-Thodos correlation [28,30] is used to determine the low pressure, pure gas viscosities for each component. This is a one time calculation and is done immediately after reading the components present in the system, using the following method

$$\mu_i = \frac{34.0 * 10^{-5} T_{R_i}^{.94}}{\tau_i}, \quad T_{R_i} \leq 1.5 \quad (3-58)$$

$$\mu_i = \frac{17.78 * 10^{-5} (4.58 T_{R_i} - 1.67)^{.625}}{\tau_i}, \quad T_{R_i} > 1.5 \quad (3-59)$$

where

$$\tau_i = \frac{5.44085 T_{C_i}^{1/6}}{M_i^{1/2} P_{C_i}^{2/3}} \quad (3-60)$$

The low pressure gas mixture viscosity is calculated first using the Herning-Zipperer equation [28,30] which has the following form

$$\mu_m = \frac{\sum y_i M_i^{1/2} \mu_i}{\sum y_i M_i^{1/2}} \quad (3-61)$$

This value is then modified to produce the actual viscosity of the mixture at reservoir conditions using the Jossi-

Stiel-Thodos correlation [28,30]

$$\begin{aligned} \mu_L = \mu_m + \{ & [(.1023 + .023364 \left(\frac{\rho_L}{\rho_{CL}} \right) + .058533 \left(\frac{\rho_L}{\rho_{CL}} \right)^2 \\ & - .040758 \left(\frac{\rho_L}{\rho_{CL}} \right)^3 + .0093324 \left(\frac{\rho_L}{\rho_{CL}} \right)^4 - .001] / \tau_L \} \end{aligned} \quad (3-62)$$

and the Dean-Stiel correlation [28,30]

$$\begin{aligned} \mu_V = \mu_m + \{ & 10.8 * 10^{-5} [\exp \left(1.439 \frac{\rho_V}{\rho_{CV}} \right) \\ & - \exp \left(-1.111 \left(\frac{\rho_V}{\rho_{CV}} \right)^{1.858} \right)] / \tau_V \} \end{aligned} \quad (3-63)$$

where the variables used are as defined in the Table of Nomenclature in Appendix A. The Lohreng [28] method, a procedure incorporating several other viscosity correlations, has been used for determining the vapor and liquid viscosities of the hydrocarbon mixtures encountered during the reservoir simulation.

CHAPTER IV

FORMULATION OF SYSTEM EQUATIONS

An integral element of any simulator is the development of the equations which describe the system. This is also true for a compositional simulator. The development of the compositional reservoir equations is not complex, but does yield bulky equations with a great many terms. To enable these equations to be presented more clearly, various short-hand notations will be introduced during the development of the system equations.

The general phase equations for a reservoir system can be written as

$$\nabla \cdot \left[A \rho_j k \left(\frac{k_r}{\mu} \right)_j \nabla \phi_j \right] - q_{vj} = \frac{\partial}{\partial t} (\phi \rho_j S_j) V_k \quad (4-1)$$

where j is a phase identifier and represents oil, gas, or water. Other variables are described in Appendix A. Also available are flow potential equations, of the form,

$$\phi_j = P_j - \rho_j gh \quad (4-2)$$

where, again, j is a phase identifier for oil, gas, or water. The water and gas phase pressures can be described by the oil phase pressure and the capillary pressures using the

relations

$$P_w = P_1 - P_{cwo} \quad (4-3)$$

$$P_g = P_1 + P_{cgo} \quad (4-4)$$

This is an area where most compositional simulators available in the literature make the simplifying assumption that the capillary pressure forces are negligible. This package will include the capillary pressure equations and will not make the assumption that all phase pressures are equal.

In addition, saturation relations are available from the definition of phase saturations which says that the sum of the saturation of each phase must be unity and, from this, that the sum of the derivatives of each phase saturation must equal zero.

These relationships provide sufficient basis for the development of a single equation which describes the compositional reservoir system. This development will now be discussed more fully.

Substituting equation (4-2) into equation (4-1), breaking up the differential on the right hand side, and dividing through by ρ_j gives a new general phase equation of the form

$$\nabla[Ak\lambda_j \nabla\phi_j] - \frac{q_{vj}}{\rho_j} = \frac{V_k}{\rho_j} \left[\phi S_j \frac{\partial \rho_j}{\partial t} + \rho_j S_j \frac{\partial \phi}{\partial t} + \rho_j \phi \frac{\partial S_j}{\partial t} \right] \quad (4-5)$$

where λ_j is the interblock mobility term.

We can use the relation

$$\frac{\partial \rho_j}{\partial t} = \frac{\partial \rho_j}{\partial P} \frac{\partial P}{\partial t} \quad (4-6)$$

to make the substitution

$$a_j = \frac{S_j}{\rho_j} \frac{\partial \rho_j}{\partial P} \quad (4-7)$$

again where j is a phase saturation identifier. Recognizing that the compressibility of a given phase is defined as

$$C = \frac{1}{\rho} \frac{d\rho}{dP} \quad (4-8)$$

we can determine the simplifying values a_j for oil, gas, and water as

$$a_j = S_j C_j \quad (4-9)$$

where C_j is input to the simulator as a function of pressure in a table of lookup or polynomial curve fit.

The general equation, upon summing the general phase equation for each of the three phases, and using the saturation relations, becomes

$$\begin{aligned} & \nabla \cdot [A \lambda_\ell \nabla (P_\ell - \rho_\ell g h) + A \lambda_w \nabla (P_w - \rho_w g h) + A \lambda_g \nabla (P_g - \rho_g g h)] \\ & - \left(\frac{q_{v\ell}}{\rho_\ell} + \frac{q_{vw}}{\rho_w} + \frac{q_{vg}}{\rho_g} \right) - V_k (a_\ell + a_w + a_g) \frac{\partial P}{\partial t} \\ & - V_k \frac{\partial \phi}{\partial t} = 0 \end{aligned} \quad (4-10)$$

By using the capillary pressure relationships, the general equation is put in a form with only the oil pressure unknown. Again incorporating variables to simplify the general

equation,

$$B_1 = a + a_w + a_g - \frac{1}{\phi} \frac{\partial \phi}{\partial P_\ell} \quad (4-11)$$

$$B_2 = \frac{q_{v\ell}}{\rho_\ell} + \frac{q_{vw}}{\rho_w} + \frac{q_{vg}}{\rho_g} \quad (4-12)$$

$$\lambda_t = \lambda_\ell + \lambda_w + \lambda_g \quad (4-13)$$

the final differential equation which describes the reservoir system is

$$\begin{aligned} & \nabla \cdot [A\lambda_t \nabla (P_\ell - \rho_\ell gh) + A\lambda_w \nabla (P_{cwo} + \rho_w gh) + A\lambda_g \nabla (P_{cgo} - \rho_g gh)] \\ & - B_2 - V_k \phi B_1 \frac{\partial P}{\partial t} = 0 \end{aligned} \quad (4-14)$$

The above equation is converted to finite difference form and analyzed using any one of several finite difference techniques which are available in the simulation package. These developments will be discussed later.

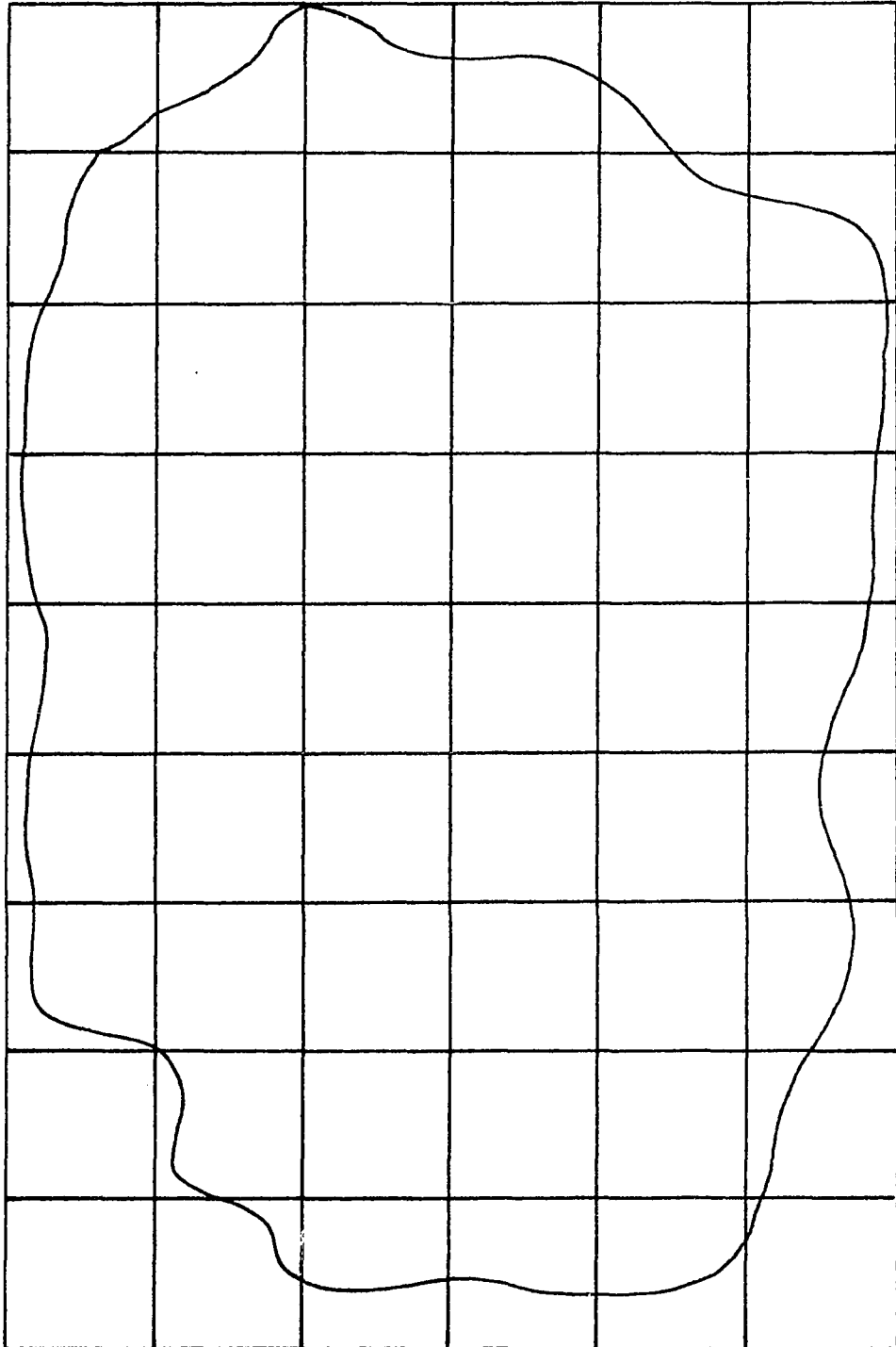
CHAPTER V

DISCRETIZATION OF RESERVOIR SYSTEM

Except for the most trivial cases the non-linear partial differential equations which relate the oil phase pressure with time throughout the porous media of the reservoir are impossible to solve analytically. Generally, the only method of solution which can be used is a numerical formulation. While an analytical approach produces a continuous solution which exactly describes any point in the system, a numerical technique produces a discrete solution which is an approximation of the exact solution for a number of points near the same location in space or time. The transformation of the continuous differential equation to a discrete form, using finite difference techniques, will be discussed in the next chapter. The transformation of the continuous reservoir system to a discretized system is a simple procedure, but does require some explanation.

The spatial reservoir system is broken up into a number of cells or blocks by overlaying a grid system. This grid system is generally, as in this simulation package, a two-dimensional rectangular form. An oddly shaped reservoir, as shown in Figure 4, is overlaid with the desired

Figure 4
Overlay of Discrete Grid System
onto Reservoir System



grid. Because of the random shape of a typical reservoir, some of the blocks of the overlayed system may not lie within the bounds of the reservoir and these are called imaginary cells. Blocks which have at least a majority of their area within the reservoir are called real cells and are assigned values which are the average value of the area within the block.

Time must also be discretized in order to be used in numerical simulation. This is done by breaking up the total time to be studied into a number of time steps. During each of these time steps, the dependent parameter is calculated which is an approximate value of the continuous function. The time step size chosen depends on the system being considered and, as would be suspected, the smaller the time step size the more accurate the solution obtained.

This grid system is then used, along with the finite difference techniques available, to solve the given reservoir system at the discrete points in the center of each cell block.

CHAPTER VI

FINITE DIFFERENCE FORMULATION

Several different finite difference techniques are made available for use in the reservoir simulation package. No one technique is superior for all reservoir systems possibly encountered. For reservoirs with large areal blocks and where directional permeabilities are approximately equal, the Alternating Direction Implicit Procedure (ADIP) is the most efficient algorithm; as the degree of anisotropy increases and the areal block sizes decrease, the ADIP method breaks down and iterative methods, such as the Line Successive Over-Relaxation (LSOR) and the Iterative Alternating Direction Implicit Procedure (IADIP) techniques, are the more efficient methods of solution for the cell pressure values.

Finite difference techniques are used to solve the non-linear partial differential equation which describes the general reservoir system. This is done by making the following substitution in the general partial differential equation:

$$\frac{\partial}{\partial x} \left[A_i \frac{\partial B_i}{\partial x} \right] = \frac{2}{\Delta x_i} \left[A_{i+\frac{1}{2}} \left(\frac{B_{i+1} - B_i}{\Delta x_{i+1} + \Delta x_i} \right) - A_{i-\frac{1}{2}} \left(\frac{B_i - B_{i-1}}{\Delta x_i + \Delta x_{i-1}} \right) \right] \quad (6-1)$$

where the variables subscripted as $i + \frac{1}{2}$ or $i - \frac{1}{2}$ are the values evaluated at the boundary between the i 'th and $i + 1$, or i 'th and $i - 1$ cells, respectively. The discretized equation is then solved using one of the several solution techniques available.

The Alternating Direction Implicit Procedure (ADIP)

This method involves dividing each time step into two equal substeps. During the first substep, the grid system is swept in the x-direction, one row at a time, solving for the unknown pressure of each cell. During the second substep, the system is swept in the y-direction, one column at a time, solving for the unknown pressure of each cell. The pressure values obtained at the end of the second substep are the pressures for the system at the $n + 1$ time level. The more complex two-dimensional problem is reduced to two one-dimensional problems.

The finite difference formulation of the general system equation is manipulated to produce the tridiagonal matrix values. During the first substep, an x-direction sweep is carried out and the pressure values of the cells in the rows above ($i + n$) and below ($i - n$) are assumed known from the most recent calculation of each cell, reducing the original five unknowns to only three unknowns. The x-direction sweep equation becomes

$$A_i p_{i-1}^{n+\frac{1}{2}} + B_i p_i^{n+\frac{1}{2}} + C_i p_{i+1}^{n+\frac{1}{2}} = D_i \quad (6-2)$$

where A_i , B_i , C_i , and D_i are as shown in Figure 5. The

Figure 5

Coefficients of x-Direction Sweep for ADIP

$$\begin{aligned}
A_i &= \frac{\theta}{\Delta x_i} \left[\frac{\lambda x t_{i-\frac{1}{2}}}{\Delta x_{t i-\frac{1}{2}}} \right] \\
B_i &= \frac{\theta}{\Delta x_i} \left[\frac{-\lambda x t_{i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}} - \frac{\lambda x t_{i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}} \right] - \frac{V_i B_{1i}}{\Delta t} \\
C_i &= \frac{\theta}{\Delta x_i} \left[\frac{\lambda x t_{i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}} \right] \\
D_i &= \frac{-\theta}{\Delta y_i} \left\{ \lambda y t_{i+\frac{1}{2}n} \frac{[(P_\ell)_{i+n} - (P_\ell)_i]}{\Delta y_{i+\frac{1}{2}n}} - \lambda y t_{i-\frac{1}{2}n} \frac{[(P_\ell)_{i+n} - (P_\ell)_i]}{\Delta y_{i-\frac{1}{2}n}} \right. \\
&+ \sum_j^{\ell, g, w} \left[\lambda y j_{i-\frac{1}{2}n} \frac{[(\rho_j gh)_i - (\rho_j gh)_{i-n}]}{\Delta y_{i-\frac{1}{2}n}} \right. \\
&- \left. \lambda y j_{i+\frac{1}{2}n} \frac{[(\rho_j gh)_{i+n} - (\rho_j gh)_i]}{\Delta y_{i+\frac{1}{2}n}} \right] + \lambda y w_{i-\frac{1}{2}n} \frac{[(P_{cwo})_i - (P_{cwo})_{i-n}]}{\Delta y_{i-\frac{1}{2}}} \\
&- \lambda y w_{i+\frac{1}{2}n} \frac{[(P_{cwo})_{i+n} - (P_{cwo})_i]}{\Delta y_{i+\frac{1}{2}n}} + \lambda y g_{i+\frac{1}{2}n} \frac{[(P_{cgo})_{i+n} - (P_{cgo})_i]}{\Delta y_{i+\frac{1}{2}n}} \\
&+ \lambda y g_{i-\frac{1}{2}n} \frac{[(P_{cgo})_i - (P_{cgo})_{i-n}]}{\Delta y_{i-\frac{1}{2}n}} - \frac{\theta}{\Delta x_i} \sum_j^{\ell, g, w} \left[\lambda x j_{i-\frac{1}{2}} \right. \\
&\times \left. \frac{[(\rho_j gh)_i - (\rho_j gh)_{i-1}]}{\Delta x_{i-\frac{1}{2}}} - \lambda x j_{i+\frac{1}{2}} \frac{[(\rho_j gh)_{i+1} - (\rho_j gh)_i]}{\Delta x_{i+\frac{1}{2}}} \right] \\
&+ \lambda x w_{i-\frac{1}{2}} \frac{[(P_{cwo})_i - (P_{cwo})_{i-1}]}{\Delta x_{i-\frac{1}{2}}} - \lambda x w_{i+\frac{1}{2}} \frac{[(P_{cwo})_{i+1} - (P_{cwo})_i]}{\Delta x_{i+\frac{1}{2}}} \\
&+ \left. \lambda x g_{i+\frac{1}{2}} \frac{[(P_{cgo})_{i+1} - (P_{cgo})_i]}{\Delta x_{i+\frac{1}{2}}} - \lambda x g_{i-\frac{1}{2}} \frac{[(P_{cgo})_i - (P_{cgo})_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \right\} \\
&+ OT_i
\end{aligned}$$

variable OT_i consists of all of the values based on the last time step and is determined from the equation shown in Figure 6.

During the second substep, a y-direction sweep is carried out and the pressure values of the cells in the columns to the left ($i - 1$) and right ($i + 1$) are assumed known from the most recent calculation of each cell. The y-direction sweep equation has three unknowns and becomes

$$A_i p_{i-n}^{n+1} + B_i p_i^{n+1} + C_i p_{i+n}^{n+1} = D_i \quad (6-3)$$

where A_i , B_i , C_i , and D_i are as shown in Figure 7. The x-direction sweep yields a close band tridiagonal matrix system when written for each cell in the model, while the y-direction sweep yields a wide band tridiagonal matrix system. The close band matrix is solved using the Thomas algorithm at the end of the x-direction sweep and the wide band matrix is solved using a modified form of the Thomas algorithm at the end of the y-direction sweep.

The Thomas algorithm is a standard technique for solving a tridiagonal matrix system and involves a forward sweep and a backward sweep of the matrix. The forward sweep for a close band matrix system involves the following procedure:

$$C_1 = C_1/B_1 \quad (6-4)$$

$$D_1 = D_1/B_1 \quad (6-5)$$

$$C_i = C_i/(B_i - A_i * C_{i-1}), \quad i = 2, n \quad (6-6)$$

$$D_i = D_i/(B_i - A_i * C_{i-1}), \quad i = 2, n \quad (6-7)$$

Figure 6

Previous Time Level Equation Used In Finite Difference Techniques

$$\begin{aligned}
OT_i = & \frac{(\theta - 1)}{\Delta x_i} \left\{ \lambda_{xt_{i+\frac{1}{2}}} \frac{[(P_\ell)_{i+1} - (P_\ell)_i]}{\Delta x_{i+\frac{1}{2}}} - \lambda_{xt_{i-\frac{1}{2}}} \frac{[(P_\ell)_i - (P_\ell)_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \right. \\
& + \sum_j^{\ell, g, w} \left[\lambda_{xj_{i-\frac{1}{2}}} \frac{[(\rho_j gh)_i - (\rho_j gh)_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \right. \\
& - \lambda_{xj_{i+\frac{1}{2}}} \frac{[(\rho_j gh)_{i+1} - (\rho_j gh)_i]}{\Delta x_{i+\frac{1}{2}}} + \lambda_{yj_{i-\frac{1}{2}n}} \frac{[(\rho_j gh)_i - (\rho_j gh)_{i-n}]}{\Delta y_{i-\frac{1}{2}n}} \\
& - \lambda_{yj_{i+\frac{1}{2}n}} \frac{[(\rho_j gh)_{i+n} - (\rho_j gh)_i]}{\Delta y_{i+\frac{1}{2}n}} \left. \right] + \lambda_{xw_{i-\frac{1}{2}}} \frac{[(P_{cwo})_i - (P_{cwo})_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \\
& - \lambda_{xw_{i+\frac{1}{2}}} \frac{[(P_{cwo})_{i+1} - (P_{cwo})_i]}{\Delta x_{i+\frac{1}{2}}} + \lambda_{xg_{i+\frac{1}{2}}} \frac{[(P_{cgo})_{i+1} - (P_{cgo})_i]}{\Delta x_{i+\frac{1}{2}}} \\
& - \lambda_{xg_{i-\frac{1}{2}}} \frac{[(P_{cgo})_i - (P_{cgo})_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \left. \right\} + \frac{(\theta - 1)}{\Delta y_i} \left\{ \lambda_{yt_{i+\frac{1}{2}n}} \right. \\
& \times \frac{[(P_\ell)_{i+n} - (P_\ell)_i]}{\Delta y_{i+\frac{1}{2}n}} - \lambda_{yt_{i-\frac{1}{2}n}} \frac{[(P_\ell)_i - (P_\ell)_{i-n}]}{\Delta y_{i-\frac{1}{2}n}} \\
& + \sum_j^{\ell, g, w} \left[\lambda_{yj_{i-\frac{1}{2}n}} \frac{[(\rho_j gh)_i - (\rho_j gh)_{i-n}]}{\Delta y_{i-\frac{1}{2}n}} \right. \\
& - \lambda_{yj_{i+\frac{1}{2}n}} \frac{[(\rho_j gh)_{i+n} - (\rho_j gh)_i]}{\Delta y_{i+\frac{1}{2}n}} \left. \right] + \lambda_{yw_{i-\frac{1}{2}}} \frac{[(P_{cwo})_i - (P_{cwo})_{i-n}]}{\Delta y_{i-\frac{1}{2}n}} \\
& - \lambda_{yw_{i+\frac{1}{2}n}} \frac{[(P_{cwo})_{i+n} - (P_{cwo})_i]}{\Delta y_{i+\frac{1}{2}n}} + \lambda_{yg_{i+\frac{1}{2}n}} \frac{[(P_{cgo})_{i+n} - (P_{cgo})_i]}{\Delta y_{i+\frac{1}{2}n}} \\
& - \lambda_{yg_{i-\frac{1}{2}n}} \frac{[(P_{cgo})_i - (P_{cgo})_{i-n}]}{\Delta y_{i-\frac{1}{2}n}} \left. \right\} + B_2 - \frac{V_i B_{1i}}{\Delta t} (P_\ell)_i
\end{aligned}$$

Figure 7

Coefficients of y-Direction Sweep for ADIP

$$\begin{aligned}
A_i &= \frac{\theta}{\Delta y_i} \left[\frac{\lambda y t_{i-\frac{1}{2}\eta}}{\Delta y_{i-\frac{1}{2}\eta}} \right] \\
B_i &= \frac{\theta}{\Delta y_i} \left[\frac{-\lambda y t_{i+\frac{1}{2}\eta}}{\Delta y_{i+\frac{1}{2}\eta}} - \frac{\lambda y t_{i-\frac{1}{2}\eta}}{\Delta y_{i-\frac{1}{2}\eta}} \right] - \frac{V_i B_{li}}{\Delta t} \\
C_i &= \frac{\theta}{\Delta y_i} \left[\frac{\lambda y t_{i+\frac{1}{2}\eta}}{\Delta y_{i+\frac{1}{2}\eta}} \right] \\
D_i &= \frac{-\theta}{\Delta x_i} \left\{ \lambda_{xt_{i+\frac{1}{2}}} \frac{[(P_\ell)_{i+1} - (P_\ell)_i]}{\Delta x_{i+\frac{1}{2}}} - \lambda_{xt_{i-\frac{1}{2}}} \frac{[(P_\ell)_i - (P_\ell)_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \right. \\
&\quad + \sum_j^{\ell, g, w} \left[\lambda_{xj_{i-\frac{1}{2}}} \frac{[(\rho_j gh)_i - (\rho_j gh)_{i-1}]}{\Delta x_{i-\frac{1}{2}}} - \lambda_{xj_{i+\frac{1}{2}}} \frac{[(\rho_j gh)_{i+1} - (\rho_j gh)_i]}{\Delta x_{i+\frac{1}{2}}} \right] \\
&\quad + \lambda_{xw_{i-\frac{1}{2}}} \frac{[(P_{cwo})_i - (P_{cwo})_{i-1}]}{\Delta x_{i-\frac{1}{2}}} - \lambda_{xw_{i+\frac{1}{2}}} \frac{[(P_{cwo})_{i+1} - (P_{cwo})_i]}{\Delta x_{i+\frac{1}{2}}} \\
&\quad + \lambda_{xh_{i+\frac{1}{2}}} \frac{[(P_{cgo})_{i+1} - (P_{cgo})_i]}{\Delta x_{i+\frac{1}{2}}} - \lambda_{xg_{i-\frac{1}{2}}} \frac{[(P_{cgo})_i - (P_{cgo})_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \Big\} \\
&\quad - \frac{\theta}{\Delta y_i} \left\{ \sum_j^{\ell, g, w} \left[\lambda_{yj_{i-\frac{1}{2}\eta}} \frac{[(\rho_j gh)_i - (\rho_j gh)_{i-\eta}]}{\Delta y_{i-\frac{1}{2}\eta}} \right. \right. \\
&\quad - \lambda_{yj_{i+\frac{1}{2}\eta}} \frac{[(\rho_j gh)_{i+\eta} - (\rho_j gh)_i]}{\Delta y_{i+\frac{1}{2}\eta}} \Big] + \lambda_{yw_{i-\frac{1}{2}\eta}} \frac{[(P_{cwo})_i - (P_{cwo})_{i-\eta}]}{\Delta y_{i-\frac{1}{2}\eta}} \\
&\quad - \lambda_{yw_{i+\frac{1}{2}\eta}} \frac{[(P_{cwo})_{i+\eta} - (P_{cwo})_i]}{\Delta y_{i+\frac{1}{2}\eta}} + \lambda_{yg_{i+\frac{1}{2}}} \frac{[(P_{cgo})_{i+\eta} - (P_{cgo})_i]}{\Delta y_{i+\frac{1}{2}\eta}} \\
&\quad \left. \left. - \lambda_{yg_{i-\frac{1}{2}\eta}} \frac{[(P_{cgo})_i - (P_{cgo})_{i-\eta}]}{\Delta y_{i-\frac{1}{2}\eta}} \right\} + OT_i
\end{aligned}$$

where n is the number of cells in the system and A , B , C , and D are the arrays of elements of the tridiagonal system as shown in Figure 8. The backward sweep is

$$D_{i-1} = D_{i-1} - C_{i-1} * D_i, \quad i = n, 1 \quad (6-8)$$

The solution to the close band tridiagonal matrix system is thus the new matrix D .

The Thomas algorithm is slightly modified to handle a wide band matrix system, one in which diagonal arrays A and C are separated from diagonal array B by one or more zero diagonals. The forward sweep becomes

$$A_i = C_i / B_i, \quad i = 1, n \quad (6-9)$$

$$D_i = D_i / B_i, \quad i = 1, n \quad (6-10)$$

$$A_i = C_i / (B_i - A_i * A_{i-n}), \quad i = n+1, n \quad (6-11)$$

$$D_i = (D_i - A_i * D_{i-n}) / (B_i - A_i * A_{i-n}), \quad i = n+1, n \quad (6-12)$$

The backward sweep is

$$D_i = D_i - A_i * D_{i-1}, \quad i = n-n, 1 \quad (6-13)$$

Again, the solution to the wide band tridiagonal matrix system is the new matrix D .

The Iterative Alternating Direction Implicit Procedure (IADIP)

This iterative method is similar to the ADI procedure discussed above but involves the addition of a term called the acceleration parameter. Beginning with the same general, two-dimensional system equation for the oil phase pressure,

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the same finite difference formulation is obtained except for the addition of the acceleration parameter term (H_k). With the addition of the acceleration parameter, the x-direction sweep equation becomes

$$A_i P_{i-1}^{n+\frac{1}{2}k+1} + B_i P_i^{n+\frac{1}{2}k+1} + C_i P_{i+1}^{n+\frac{1}{2}k+1} = D_i \quad (6-14)$$

where A_i and C_i are the same as defined for the x-direction sweep of the ADI procedure and

$$B_i = B_i(x\text{-ADIP}) - H_k \quad (6-15)$$

$$D_i = D_i(x\text{-ADIP}) - H_k [P_\ell]_i^n \quad (6-16)$$

The close band form of the Thomas algorithm is again used to solve the generated tridiagonal matrix system.

The y-direction sweep equation becomes

$$A_i P_{i-\eta}^{n+1k+1} + B_i P_i^{n+1k+1} + C_i P_{i+\eta}^{n+1k+1} = D_i \quad (6-17)$$

where

$$B_i = B_i(y\text{-ADIP}) - H_k \quad (6-18)$$

$$D_i = D_i(y\text{-ADIP}) - H_k [(P_\ell)_i^n] \quad (6-19)$$

and A_i and C_i are as defined in the y-direction sweep of the ADI procedure. The tridiagonal matrix system is solved, as before, using the wide band form of the Thomas algorithm

The successive iterative use of a set of acceleration parameters constitutes a cycle. Equations (6-14) and (6-17) are solved iteratively, using a different acceleration

parameter for each iteration. At the end of each cycle a relative error check is made.

An optimal set of acceleration parameters is necessary to achieve the superior efficiency of this method. The determination of a set of optimum acceleration parameters is difficult analytically and is usually achieved using trial and error techniques. The upper and lower limits of the parameter can be estimated using the method of Peaceman and Rachford [31]. It has been pointed out that a geometric series of acceleration parameters produces optimum results [31]. A subroutine to estimate the acceleration parameters is available to the operator of this simulator and is discussed more fully in Chapter VII.

The acceleration parameters must be normalized to account for possible differences in the areal size of any one cell of the model with respect to the others.

$$H_k = H_k \lambda_i \quad (6-20)$$

$$\lambda_m = \left(\frac{1}{n} \sum_{i=1}^n K_i \right) \left(\frac{.22}{\Delta x_m \Delta y_m} \right) \quad (6-21)$$

The acceleration parameters are normalized within the IADIP computation.

Line Successive Over-Relaxation (LSOR)

This method is similar to the ADI procedure except that a solution sweep of the model occurs in one direction rather than two. The system is swept in the x-direction, row by row. Beginning with the general, two-dimensional

form of the pressure equation, the finite difference form of the equation is identical to that obtained for the ADI procedure. With only one time substep, the x-direction sweep becomes

$$A_i p_{i-1}^{k+1} + B_i p_i^{k+1} + C_i p_{i+1}^{k+1} = D_i \quad (6-22)$$

where A_i , B_i , C_i , and D_i are as given in Figure 9. The variable OT_i is a combination of all values based on the previous time step and is shown in Figure 7.

At the completion of each sweep of the system, if the relative error check is not satisfied, the updated pressure estimates are over-relaxed to produce more accurate updated values.

$$p_i^{k+1} = p_i^k + \omega(p_i^{k+1} - p_i^k) \quad (6-23)$$

An optimum relaxation parameter (ω) is necessary for maximum efficiency of this method. The selection of this optimum value requires a trial and error approach. Several abbreviated simulation runs are made with various relaxation parameters. The number of iterations required for convergence is then plotted versus the relaxation parameter. A typical plot of this relationship is shown in Figure 10. This graph has the characteristic shape of a cusp, with the low point of this cusp being the optimum relaxation parameter. As a general rule, the more homogeneous the system, the closer the value of the relaxation parameter is to 1.0, while

Figure 9

Coefficients Used in the LSOR Procedure

$$\begin{aligned}
A_i &= \frac{\theta}{\Delta x_i} \left[\frac{\lambda x t_{i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}} \right] \\
B_i &= \frac{\theta}{\Delta x_i} \left[\frac{-\lambda x t_{i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}} - \frac{\lambda x t_{i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}} \right] - \frac{\theta}{\Delta y_i} \left[\frac{\lambda y t_{i+\frac{1}{2}n}}{\Delta y_{i+\frac{1}{2}n}} + \frac{\lambda y t_{i-\frac{1}{2}n}}{\Delta y_{i-\frac{1}{2}n}} \right] - \frac{V_i B_{1i}}{\Delta t} \\
C_i &= \frac{\theta}{\Delta x_i} \left[\frac{\lambda x t_{i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}} \right] \\
D_i &= \frac{-\theta}{\Delta y_i} \left\{ \lambda y t_{i+\frac{1}{2}} \frac{(P_\ell)_{i+n}}{\Delta y_{i+\frac{1}{2}n}} + \lambda y t_{i-\frac{1}{2}n} \frac{(P_\ell)_{i-n}}{\Delta y_{i-\frac{1}{2}n}} + \sum_j^{\ell, g, w} \left[\lambda y j_{i-\frac{1}{2}n} \right. \right. \\
&\quad \times \left. \frac{[(\rho_j gh)_i - (\rho_j gh)_{i+n}]}{\Delta y_{i-\frac{1}{2}n}} - \lambda y j_{i+\frac{1}{2}n} \frac{[(\rho_j gh)_{i+n} - (\rho_j gh)_i]}{\Delta y_{i+\frac{1}{2}n}} \right] \\
&\quad + \lambda y w_{i-\frac{1}{2}n} \frac{[(P_{cwo})_i - (P_{cwo})_{i-n}]}{\Delta y_{i-\frac{1}{2}n}} - \lambda y w_{i+\frac{1}{2}n} \frac{[(P_{cwo})_{i+n} - (P_{cwo})_i]}{\Delta y_{i+\frac{1}{2}n}} \\
&\quad + \lambda y g_{i+\frac{1}{2}n} \frac{[(P_{cgo})_{i+n} - (P_{cgo})_i]}{\Delta y_{i+\frac{1}{2}n}} - \lambda y g_{i-\frac{1}{2}n} \frac{[(P_{cgo})_i - (P_{cgo})_{i-n}]}{\Delta y_{i-\frac{1}{2}n}} \Big\} \\
&\quad - \frac{\theta}{\Delta x_i} \left\{ \sum_j^{\ell, g, w} \left[\lambda x j_{i-\frac{1}{2}} \frac{[(\rho_j gh)_i - (\rho_j gh)_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \right. \right. \\
&\quad - \lambda x j_{i+\frac{1}{2}} \frac{[(\rho_j gh)_{i+1} - (\rho_j gh)_i]}{\Delta x_{i+\frac{1}{2}}} \Big] + \lambda x w_{i-\frac{1}{2}} \frac{[(P_{cwo})_i - (P_{cwo})_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \\
&\quad - \lambda x w_{i+\frac{1}{2}} \frac{[(P_{cwo})_{i+1} - (P_{cwo})_i]}{\Delta x_{i+\frac{1}{2}}} + \lambda x g_{i+\frac{1}{2}} \frac{[(P_{cgo})_{i+1} - (P_{cgo})_i]}{\Delta x_{i+\frac{1}{2}}} \\
&\quad \left. \left. - \lambda x g_{i-\frac{1}{2}} \frac{[(P_{cgo})_i - (P_{cgo})_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \right\} + OT_i
\end{aligned}$$

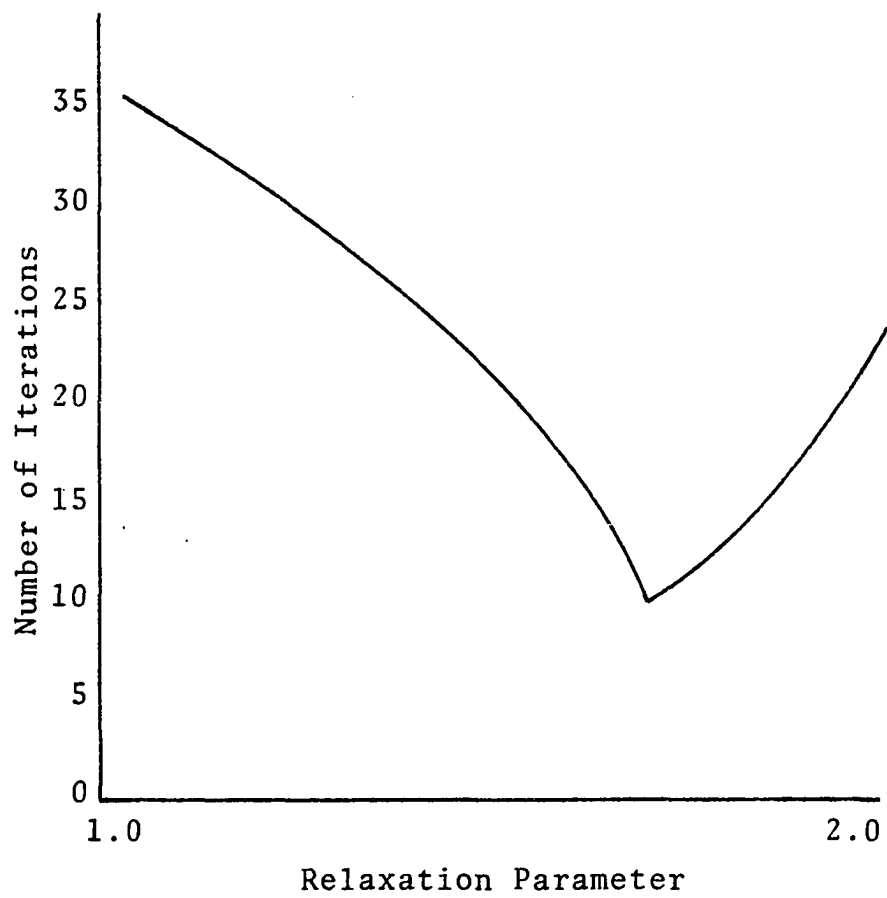


Figure 10
Typical Plot of Relaxation Parameter

the value approaches 2.0 as the degree of anisotropy of the system increases. As can be seen from Figure 10, an over-estimation of the relaxation parameter is always preferred to an underestimation.

These three finite difference solution techniques, ADIP, IADIP, and LSOR, are programmed such that the user has the option of choosing the solution technique to be used to solve the oil phase pressure equation.

CHAPTER VII

AUXILIARY PORTIONS OF SIMULATION PACKAGE

A number of auxiliary routines have been included in the simulation package, developed either out of necessity or simply for the convenience of the engineer who digitizes the data and analyzes the results. Each of these routines will now be discussed in detail. Flow charts for these routines and all others used in this simulation package are presented in Appendix C.

WRTMOD

This routine produces a sketch, similar to that presented in Figure 11, of the system under study. When an odd shaped reservoir is discretized for analysis in a simulator, as was discussed in Chapter V, often some of the rectangular cells are not within the bounds of the system. In addition, each of the cells in the system are numbered as they are identified by the simulator. The dimensions of each cell are also shown: the x-direction dimension across the top of the sketch and the y-direction dimension down the left side.

NUMBERING SCHEME OF RESERVOIR MODEL (IMAGINARY CELLS SHADED)

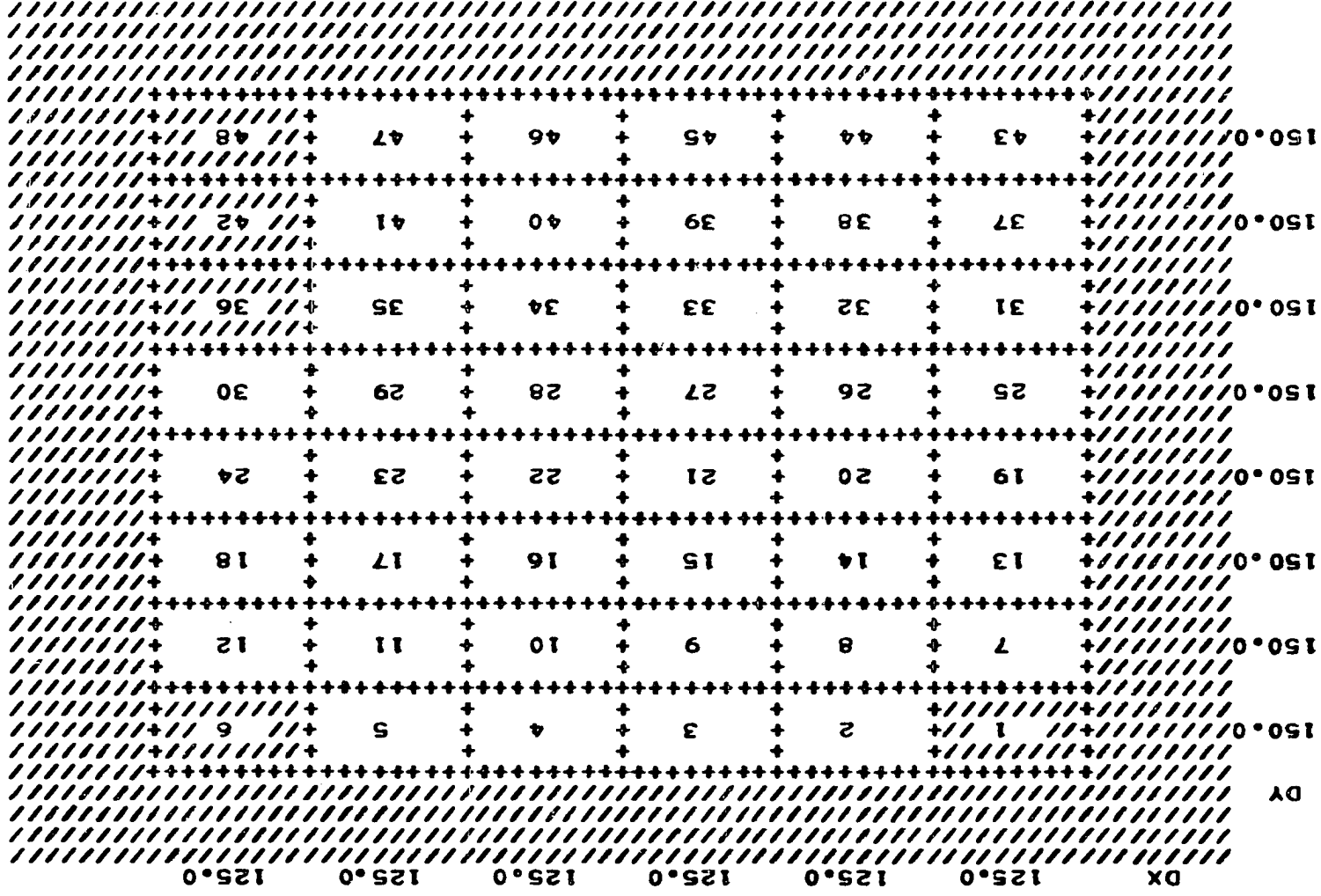


FIGURE 11

This routine serves as a check for the engineer that the discretized grid has the desired shape and provides a convenient way for him to rapidly identify separate simulation runs on several different reservoir configurations.

Information required for this routine is the x and y dimensions for each cell, the number of columns in the system, the total number of cells in the system, and the cell numbers of those cells which are outside the actual boundaries of the system.

ACCP

This routine provides the option for the user to call upon the simulation package to estimate the proper acceleration parameters to be used in the Iterative Alternating Direction Implicit Procedure (IADIP). The procedure used to obtain these estimates of acceleration parameters is outlined by Crichlow [31].

Four parameters are defined as functions of the x- and y-direction interblock transmissibilities (T_x and T_y) and the number of cells in the x- and y-direction (N_x and N_y) in the following manner

$$M_1 = \frac{2T_x}{T_x + T_y} \frac{\pi^2}{4N_x^2} \quad (7-1)$$

$$M_2 = \frac{2T_x}{T_x + T_y} \quad (7-2)$$

$$M_3 = \frac{2T_y}{T_x + T_y} \frac{\pi^2}{4N_y^2} \quad (7-3)$$

$$M_4 = \frac{2T_y}{T_x + T_y} \quad (7-4)$$

The lower limit of the acceleration parameters is the smaller of M_1 and M_3 while the upper limit is the larger of M_2 and M_4 . Birkoff, Varga, and Yound [32] point out that the acceleration parameters should be in a geometric series such that each element in the series is a constant multiplied by the previous element. The constant multiplier is determined as

$$r = \exp \left[\frac{\ln(H_m/H_1)}{M-1} \right] \quad (7-5)$$

where H_1 and H_m are the minimum and maximum acceleration parameters, respectively, and M is the number of acceleration parameters in the system. Each of the acceleration parameters can now be determined by multiplying the previous value by the constant.

This procedure is only a method of estimating the proper acceleration parameters to be used. The user must experiment to some extent in order to obtain an adequate lower value. The rate of convergence is very sensitive to this value and a slight difference in the lower acceleration parameter could result in divergence rather than convergence.

INPUT

This routine provides a means of reading a data matrix into the simulator, assigning a value to each cell of the system, and checking that the value assigned is within

the range specified for all of the matrix values. In addition, the entire matrix can be multiplied by a given factor. This latter feature is very important when one is attempting to obtain a history match in order to provide a realistic contour map of the rock properties for the system. The data matrix is written out to aid the user and any cell data which has been misspunched and lies outside the range specified for the system is printed out so that it can be easily corrected.

INDATA

The purpose of this routine is to read that data which is available as a table of lookup or a polynomial. If the data is in the form of a table of lookup, the independent and dependent variables are read and printed and an error message is provided if the independent variables in the table of lookup are not in ascending order. If the data is available in the form of a polynomial curve fit, the coefficients are read in order of increasing degree, beginning with the coefficient of the zero'th degree term. Flags are also associated with the data to indicate whether they are for a polynomial equation, a two point linear interpolation table of lookup, or a three point Lagrangian table of lookup and for the number of coefficients or sets of independent and dependent values which are provided. Tables of lookup or polynomial curve fits are typically used to describe relative permeabilities or formation volume factors which are required in a simulation package.

LOOKUP

This routine is designed to determine, given the value of the independent variable, the respective value of the dependent variable from a table of lookup or polynomial equation. The polynomial coefficients or table of lookup information are read into the simulation package using subroutine INDATA and subroutine LOOKUP determines from the appropriate flag which procedure is to be used to determine the dependent variable value desired. Either a two point linear interpolation or a three point Lagrangian interpolation procedure is available for use on table of lookup data. If the independent value submitted is out of the range of the table of lookup, an error message is printed and execution of the simulator is terminated at that point.

SORSNK

This routine provides a means for determining the flow rate at source or sink cells. The two basic wellbore conditions are flow at constant pressure conditions or flow at a constant rate. This simulation package is designed to utilize the explicit production procedure which requires that the oil, gas, and water flow rates be known a priori in order to set up the complete finite difference formulation. The explicit production formulation has the disadvantage that saturation oscillations or fluctuations in the flow rates can be produced if small grid blocks are used, large time steps are required, the reservoir exhibits a converging

flow pattern (i.e., fractures or other communications are present which increase flow rates abnormally), or extremely high production or injection rates are present. The implicit production procedure, which requires that the three phase flow rates be included in the implicit formulations of the finite difference equations, provides a safer method of handling the flow rates, but requires greater computer storage and longer execution of the simulation package. As long as the user is aware of the limitations imposed by the explicit procedure, only minimal, if any, oscillation problems should be encountered.

The formulation used in the simulation package requires either the flowing bottom hole pressure of the well or the phase volume produced of one phase, the oil, gas, or water phase, in that order. If the gas phase is given, for example, the oil phase flow rate is assumed to be zero and the water phase flow rate is calculated based on the mobility ratios and the given gas flow rate. If the flowing bottom hole pressure is given, the oil phase flow rate is calculated using the following equation:

$$q_o = \frac{7.07 k_{ro} Kh(\bar{P} - P_{wf})}{\mu_o B_o \left[\ln \left(\frac{1}{r_w} \sqrt{\frac{\Delta x \Delta y}{\pi}} \right) - \frac{3}{4} + S \right]} \quad (7-6)$$

where \bar{P} is the average cell pressure and r_w is the wellbore radius and is assumed to be .667 feet for all wells.

The new time level flow rates are calculated from the following set of equations:

$$q_o^{n+1} = q_o \quad (7-7)$$

$$q_g^{n+1} = \frac{k_{rg}}{\mu_g B_g} \frac{\mu_o B_o}{k_{ro}} q_o^{n+1} \quad (7-8)$$

$$q_w^{n+1} = \frac{k_{rw}}{\mu_w B_w} \frac{\mu_g B_g}{k_{rg}} q_o^{n+1} \quad (7-9)$$

BOUND

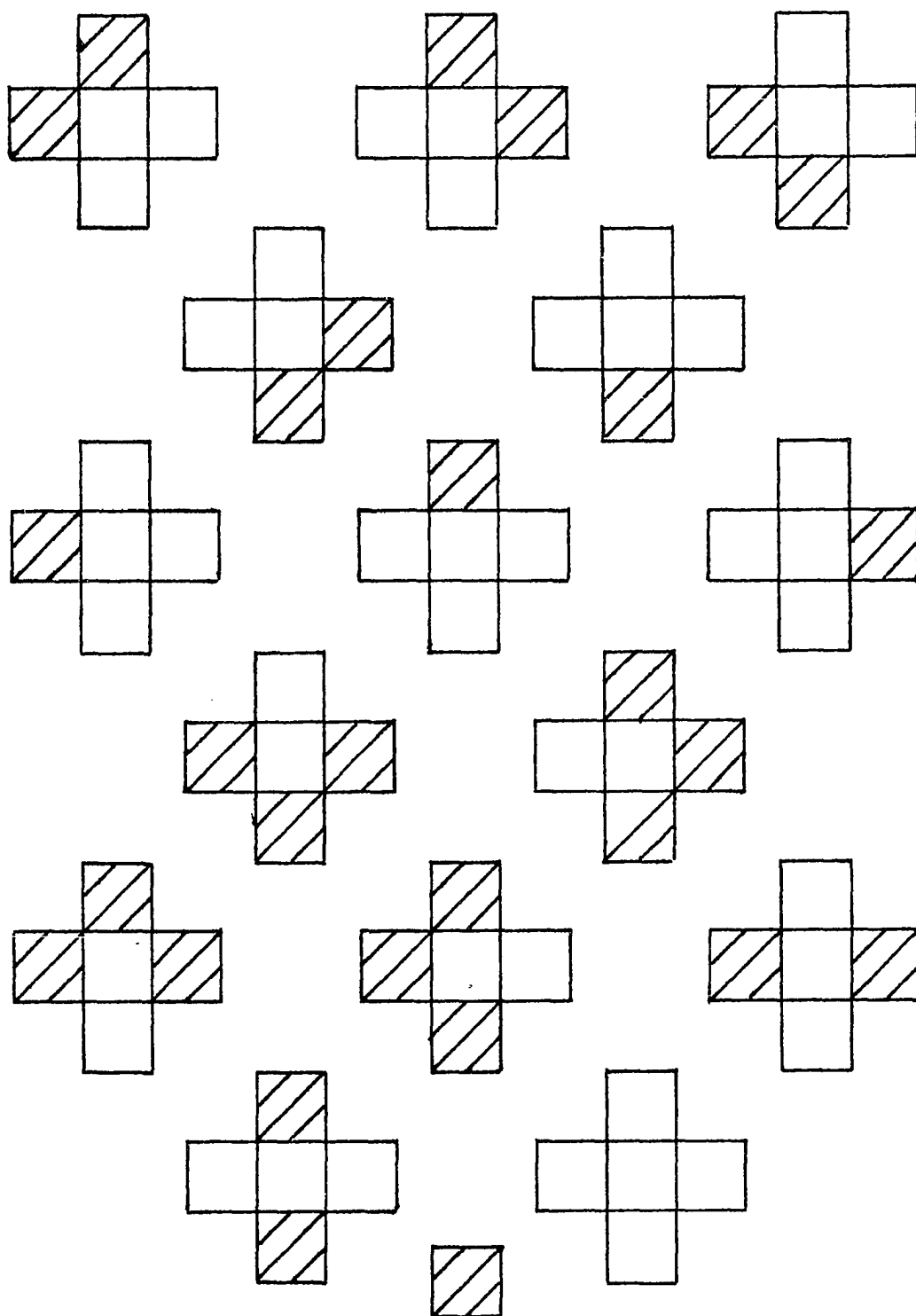
This routine examines a given cell and determines, from its position in the grid system, what values should be used in the finite difference equation for each of the four surrounding cells. This is necessary, for example, when one or more of the cell boundaries lie on the system boundary. If the given cell is not completely surrounded by other cells in the system, boundary conditions must be satisfied such that there is no flow across the system boundaries. The values used for real cells surrounding the cell of interest are the values of the surrounding cells, but, for imaginary cells surrounding the cell of interest, the value of the cell of interest is used to ensure no flow to or from any imaginary cells.

Each of the cells in the system is assigned an identifying number which indicates the configuration of it and the four surrounding cells. There are sixteen possible configurations and they are presented in Figure 12.

CUBEQN

This routine, required for use in the liquid volume correlations discussed previously, provides the smallest

Figure 12
Possible Cell Configurations



positive real root to a given cubic equation. The procedure, as outlined in the CRC Standard Mathematical Tables [14], is very simple.

The given cubic equation must be in the form

$$y^3 + Py^2 + Qy + R = 0 \quad (7-10)$$

and is reduced to the form

$$x^3 + ax + b = 0 \quad (7-11)$$

where

$$a = \frac{1}{3} (3Q - P^2) \quad (7-12)$$

$$b = \frac{1}{27} (2P^3 - 9PQ + 27R) \quad (7-13)$$

$$x = y + \frac{P}{3} \quad (7-14)$$

The smallest root of the original equation becomes

$$y = A + B - \frac{P}{3} \quad (7-15)$$

where

$$A = \left(-\frac{b}{2} + \sqrt{\frac{b^2}{4} + \frac{a^3}{27}} \right)^{1/3} \quad (7-16)$$

$$B = \left(-\frac{b}{2} - \sqrt{\frac{b^2}{4} + \frac{a^3}{27}} \right)^{1/3} \quad (7-17)$$

However, if the term inside the square root portion of A and B is less than or equal to zero, the square root is imaginary and a conjugate imaginary root to the cubic equation is produced. In this case, a trigonometric method is necessary to determine the smallest positive real root of the given equation, because an imaginary fluid volume

has no physical significance. The solution obtained from the trigonometric method has the form

$$y = 2 \sqrt{\frac{-a}{3}} \cos \left[\frac{1}{3} \cos^{-1} \left(\frac{3b}{a\sqrt{-a/3}} \right) + \frac{2}{3}\pi \right] - \frac{P}{3} \quad (7-18)$$

IBMOB1 and IBMOB2

These two routines combine to calculate the inter-block mobility ratios for each of the three phases. The equation developed by Stone [33] is used to define the relative permeability to oil as

$$k_{ro} = (k_{row} + k_{rw})(k_{rog} + k_{rg}) - (k_{rw} + k_{rg}) \quad (7-19)$$

This procedure incorporates the theory of channel flow in porous media with probability concepts to obtain a means of determining the relative permeability to oil in the presence of flowing water and gas. No simulation packages in the literature provide a means of allowing for differences in the relative permeability to oil as a result of other flowing phases being present. All of the information required for use in the Stone [33] equation is generally available as a result of reservoir core and fluid property analyses. This method provides a good fit to experimental data except in situations where a high water saturation and low gas saturation are present.

The appropriate phase permeability is modified in IBMOB2 to correspond to an upstream interblock value which is weighted by cell size. The upstream weighting method

is an extrapolation of the phase permeabilities of two upstream cells to the interblock location desired. This value is then used in the interblock mobility equation

$$\lambda_{ji} = \frac{k_{rj}}{\mu_{ji}} \quad (7-20)$$

where i is the cell indicator and j indicates the phase under consideration. Each cell mobility is multiplied at this point by the cell transmissibility value, which is a term consisting of all of the general pressure equation terms which are constant for all cells at any point in time. The transmissibility value is calculated in the mainline of the simulator as

$$Kh_x = \frac{\frac{K_i h_i \Delta y_i}{\Delta x_i} + \frac{K_{i+1} h_{i+1} \Delta y_{i+1}}{\Delta x_{i+1}}}{\Delta x_i + \Delta x_{i+1}} \quad (7-21)$$

$$Kh_y = \frac{\frac{K_i h_i \Delta x_i}{\Delta y_i} + \frac{K_{i+1} h_{i+1} \Delta x_{i+1}}{\Delta y_{i+1}}}{\Delta y_i + \Delta y_{i+1}} \quad (7-22)$$

The mobility value of each cell is replaced by the upstream mobility for the right side boundary (in the x-direction) or the bottom side boundary (in the y-direction) for the given cell. The print indicator for the interblock mobility ratio is checked and if it is any value other than zero, the matrices are printed for examination by the user. Six interblock mobility matrices are printed, each of the three phases (oil, gas, and water) in each of the two directions (x and y).

SATRN

This routine calculates the new phase saturations using the equation developed from the equations describing the reservoir system. Beginning with the phase equations, discussed in Chapter IV, and including the potential equations, we have

$$\nabla [A \rho_j k \left(\frac{k_r}{\mu} \right)_j \nabla (P_j - \rho_j g h)] - q_{vj} = \frac{\partial}{\partial t} (V_k \phi \rho_j S_j) \quad (7-23)$$

where j is the phase identifier. Breaking up the right hand side and multiplying the equation by $1/\rho_j$, we obtain

$$\nabla [A \lambda_j \nabla (P_j - \rho_j g h)] - \frac{q_{vj}}{\rho_j} - \frac{V_k}{\rho_j} [\phi S_j \frac{\partial \rho_j}{\partial t} + \rho_j S_j \frac{\partial \phi}{\partial t}] = V_k \phi \frac{\partial S_j}{\partial t} \quad (7-24)$$

where λ has been used to replace the interblock mobility ratio term.

Because the updated saturations are required to determine the new overall compositions of each cell, and the updated compositions are necessary to determine the new phase densities, it is assumed that the density change with respect to time is zero and these terms fall out of the above equation. Using finite difference techniques to discretize the new saturation equation, we have

$$\begin{aligned} S_j^{n+1} = & \frac{\Delta t}{V_i \Delta x_i} [A_x \lambda_{xj,i+1} (P_{j,i+1} - P_{j,i}) - A_x \lambda_{xj,i-1} (P_{j,i} - P_{j,i-1})] \\ & + \frac{\Delta t}{V_i \Delta y_i} [A_y \lambda_{yj,i+n} (P_{j,i+n} - P_{j,i}) - A_y \lambda_{yj,i-n} (P_{j,i} - P_{j,i-n})] \\ & - \frac{q_{vj} \Delta t}{\rho_j V_i} - \frac{S_j^n \Delta t}{\phi^n} [\phi^{n+1} - \phi^n] + S_j^n \end{aligned} \quad (7-25)$$

This equation is used to find the oil and water saturations of each cell, but the gas saturation is determined from the definition of saturation which says that the three phase saturations must sum to unity. Because of the compressibility of gas mixtures, any error which results from not using the phase saturation for the gas phase is reduced. The mass of the gas phase present in the system is not as dependent on the gas saturation as it is on the system pressure, so a gas saturation is not as critical in the phase material balance check.

UPDATE

This routine updates saturations, compositions, and fluid properties to the new pressure levels obtained from a finite difference solution of the general, oil-phase equation for the reservoir system. In addition, new phase potentials and the new overall composition matrices can be printed if the print identifier for each is some value other than zero.

The updating of the overall compositions is accomplished using finite difference techniques and the relation

$$\nabla \cdot [A \lambda_t \nabla \phi_\ell] \rho_\ell x_i + \nabla \cdot [A \lambda_t \nabla \phi_g] \rho_g y_i = V_k \frac{\partial}{\partial t} [\phi (S_\ell \rho_\ell + S_g \rho_g) z_i]$$

The final relation used to determine the new compositions for each cell is presented in Figure 13. These new overall composition values are flashed to determine the individual phase compositions and the new pressure level fluid properties are computed.

Figure 13

Equation for Updated Compositions

$$\begin{aligned}
Z_i^{n+1} = & \frac{1}{S_{\ell}^{n+1} \rho_{\ell}^n + S_g^{n+1} \rho_g^n} \left\{ (S_{\ell} \rho_{\ell} + S_g \rho_g)^n Z_i^n \right. \\
& + \frac{\Delta t}{V_i} \left[\frac{A_{x \ell} \rho_{\ell} X_i}{\Delta x_i} \left(\lambda_{xt_{i+\frac{1}{2}}} \frac{[(\phi_{\ell})_{i+1} - (\phi_{\ell})_i]}{\Delta x_{i+\frac{1}{2}}} - \lambda_{xt_{i-\frac{1}{2}}} \frac{[(\phi_{\ell})_i - (\phi_{\ell})_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \right) \right. \\
& + \frac{A_{y \ell} \rho_{\ell} X_i}{\Delta y_i} \left(\lambda_{yt_{i+\frac{1}{2}\eta}} \frac{[(\phi_{\ell})_{i+\eta} - (\phi_{\ell})_i]}{\Delta y_{i+\frac{1}{2}\eta}} - \lambda_{yt_{i-\frac{1}{2}\eta}} \frac{[(\phi_{\ell})_i - (\phi_{\ell})_{i-\eta}]}{\Delta y_{i-\frac{1}{2}\eta}} \right) \\
& + \frac{A_{x g} \rho_g Y_i}{\Delta x_i} \left(\lambda_{xt_{i+\frac{1}{2}}} \frac{[(\phi_g)_{i+1} - (\phi_g)_i]}{\Delta x_{i+\frac{1}{2}}} - \lambda_{xt_{i-\frac{1}{2}}} \frac{[(\phi_g)_i - (\phi_g)_{i-1}]}{\Delta x_{i-\frac{1}{2}}} \right) \\
& \left. \left. + \frac{A_{y g} \rho_g Y_i}{\Delta y_i} \left(\lambda_{yt_{i+\frac{1}{2}\eta}} \frac{[(\phi_g)_{i+\eta} - (\phi_g)_i]}{\Delta y_{i+\frac{1}{2}\eta}} - \lambda_{yt_{i-\frac{1}{2}\eta}} \frac{[(\phi_g)_i - (\phi_g)_{i-\eta}]}{\Delta y_{i-\frac{1}{2}\eta}} \right) \right] \right\}
\end{aligned}$$

CHAPTER VIII

RESULTS AND RECOMMENDATIONS

In order to verify the simulation package which was developed, a one-dimensional system was studied. The system consists of ten rectangular cells, each of which is one foot by 175 feet and 25 feet thick. Production from the system is out of an end cell (#1) at a flowing pressure of 1500 pounds per square inch. The initial pressure in the system is 2021 psia. The overall hydrocarbon composition is initially as follows:

Methane	0.5043
Ethane	0.1549
Propane	0.0875
Iso-Butane	0.0236
N-Butane	0.0353
Pentane	0.0295
Hexane	0.0229
Heptane	0.1420

The time step size chosen for this study is 0.05 days, and the system response was studied for 10.0 days. The pressure distribution obtained during this simulation study is presented in Table 4.

TABLE 4
Pressure Response of Test Case

Time	Cell #1	Cell #2	Cell #3	Cell #4
0.0	2021.	2021.	2021.	2021.
0.5	1775.	2016.	2021.	2021.
1.0	1735.	2007.	2021.	2021.
1.5	1716.	1996.	2020.	2021.
2.0	1708.	1985.	2020.	2021.
2.5	1705.	1974.	2019.	2021.
3.0	1706.	1964.	2018.	2021.
3.5	1708.	1954.	2017.	2021.
4.0	1713.	1945.	2016.	2021.
4.5	1717.	1937.	2015.	2021.
5.0	1723.	1930.	2014.	2021.
5.5	1729.	1923.	2012.	2020.
6.0	1734.	1917.	2011.	2020.
6.5	1740.	1911.	2009.	2020.
7.0	1746.	1906.	2008.	2020.
7.5	1751.	1902.	2006.	2020.
8.0	1756.	1898.	2004.	2020.
8.5	1761.	1894.	2002.	2019.
9.0	1766.	1891.	2001.	2019.
9.5	1770.	1888.	1999.	2019.
10.0	1775.	1886.	1997.	2018.

As can be seen by the pressure distributions, the simulation produces results which are reasonable based on our experience. As fluids are produced out of the end cell of the system, the pressure within that cell decreases. This produces a response in the next cell when the pressure drop across the boundary is sufficiently high to cause flow between the cells.

For testing purposes, it is assumed that only the oil phase was being produced from the reservoir. This results in a decrease in the oil saturation for the producing cell which in turn leads to a decrease in the relative permeability to oil and a decrease in oil production from the cell. The production eventually decreases to the point that influx into the cell continues at a greater rate than oil is being produced. A less mobile oil phase is also entering the cell but at a rate less than the production demand. The cell pressure increases due to the increasing influx of fluid; however, oil production continues to decrease. This explains the increase in pressure in cell one beginning at 45 days. The other cell pressures continue to decline as fluids move to the low pressure region.

Several weaknesses were found in the simulation package during the verification process. These will be discussed more fully.

K-Value Algorithm

The K-value algorithm used in this simulation package is felt to be a potential source of error. The deviations

evidenced during the developmental investigation also appear in a comparison of NGPSA K-values to those calculated for the test case at initial conditions:

<u>NGPSA</u>	<u>Test Case</u>
2.0	1.55
1.08	1.11
.88	.77
.64	.63
.58	.59
.40	.46
.25	.41
.16	.37

The K-value algorithm should be the area of primary concern in future studies based on this work. A relatively simple, yet very accurate, correlation must be used. A great deal of multicomponent real system data should be gathered and fit to a function of the critical properties of the individual components, the convergence pressure, and the system pressure and temperature. This data should primarily cover the range of pressures and compositions typically encountered in a petroleum reservoir in order to provide a correlation which is most accurate in the range needed. Special attention should be paid to accuracy and efficiency. An improved algorithm can be easily inserted in place of the current procedure.

Injection and Production

A second weakness in this package is the subroutine which determines the injection or production rates. The production rates computed for the one-dimensional system under study were larger than expected. This possible error should be studied, and it would be valuable to include a procedure to determine the compositions of each phase from the surface separators, taking into account the continuous flashing as a result of decreases in pressure and temperature as the fluid moves up the wellbore.

Fluid Properties

The viscosity and density correlations do not appear to cause significant errors in this particular study. In the area of the critical point of a given system these correlations deviate from reality. At the critical point of normal butane, for example, the viscosity and density correlations produce the following results:

	<u>Liquid</u>	<u>Vapor</u>
Density (lb./ft ³)	57.6	1.059
Viscosity (cp)	141.5	0.011

The liquid and vapor phase properties should be identical at the critical point. Although these results indicate a very large error at the critical point, accuracy figures presented by the authors of the various procedures show that the correlations predict real behavior very well in the wide temperature and pressure regions encountered in a petroleum reservoir. The large divergence from real behavior at the

critical point is a regional error and probably significant only at system conditions within a few units of the critical point. Inaccuracies in the region of the critical point are not intolerable because of the accuracy displayed in other regions, as long as the package user is aware of this possible source of error.

Improvements in the viscosity and density algorithms will result in a more flexible system. Before such improvements are made, the accuracy of these algorithms should be more thoroughly studied to determine if the region of error is large enough to justify the effort involved in improvements.

Conclusions

1. Of the four different types of petroleum fluids which have been discussed, the gas condensate and volatile oil reservoirs experience significant phase change effects during depletion. The black oil model, which lacks the essential features to handle transfer of mass between phases, is inadequate for predicting the behavior of these systems. A compositional approach is necessary to accurately predict the performance of petroleum reservoir systems which exhibit significant interphase mass transfer.

2. Fluid flow in porous media and thermodynamic equilibrium behavior of reservoir fluids are coupled to produce a workable mathematical model for compositional systems. This mathematical model is verified for the one-dimensional case.

3. Versatility in the numerical techniques utilized in the mathematical model is required to accommodate the different reservoir geometries and well configurations encountered in petroleum

reservoir systems. The simulation package developed incorporates this versatility by providing the option of utilizing either the Alternating Direction Implicit Procedure, the Iterative Alternating Direction Implicit Procedure, or the Line Successive Over-Relaxation Procedure to solve the reservoir system equation.

4. A prominent conclusion of this research is the indication that fast and accurate correlations for the equilibrium K-value and the system fluid properties are required to expedite the compositional simulation.

5. Efforts to minimize computer storage have produced a model which requires less than 200,000 bytes of storage in order to handle the compositional reservoir simulation of a 500-cell, ten component system. The literature provides no information on the computer storage required for similar packages.

6. Although the simulation package developed is more complex mathematically, it displays a computational superiority to other packages discussed in the literature. MacDonald [8] uses a CDC 6600 computer and reports execution times of 0.02 second/cell/component/iteration for a one-dimensional system. In contrast, this package, using an IBM 370/158 computer system, performed a one-dimensional study which required 0.002 seconds/cell/component/iteration.

In this research, a model has been developed in which capillary forces have been considered and three-phase flow permeabilities have been included to provide a prediction method which closely approaches real reservoir behavior. Storage and computational considerations have produced an economically competitive package.

APPENDICES

APPENDIX A

Nomenclature

A, B, C, D	elements of tridiagonal matrix system from finite difference techniques
A_i	cross-sectional area to flow in i'th direction
A_{mn}	element of 6 * 6 matrix of coefficients for vapor density correlation
B	formation volume factor of given phase
$f(L)$	flash function evaluated at overall liquid phase mole fraction
$f'(L)$	derivative of flash function
g	gravity
h	thickness of cell
H_k	acceleration parameter for IADIP
k	absolute permeability
k_r	relative permeability to given phase
K_i	equilibrium constant for i'th component in vapor-liquid system
L	mole fraction of system in liquid phase
M_{AV}	system average molecular weight
M_i	molecular weight of i'th component
P	system pressure
P_{cgo}	capillary pressure to oil
P_{cwo}	capillary pressure to water

P_{conv}	convergence pressure of given system
P_c	critical pressure
P_i	pressure of i'th cell
P_j	pressure of given phase
P_m	Legendre polynomial of degree 0 through 5
P_R	reduced pressure
P_{RS}	reduced component vapor pressure
P_{wf}	flowing bottom hole pressure of well
q	phase flow rate as production or injection
R	universal gas constant
S	skin effect due to wellbore damage
S	phase saturation of phase of interest
t	time
T	system temperature
T_c	critical temperature
T_R	reduced temperature
V_i	pore volume of i'th cell
V_k	bulk volume of cell
V	volume of liquid or vapor system
V	mole fraction of system in vapor phase
W_i	weight fraction of i'th component
Δx	x dimension of the given cell
x_i	mole fraction of i'th component in liquid phase
Δy	y dimension of the system
y_i	mole fraction of i'th component in vapor phase
z_i	overall mole fraction of i'th component present in vapor-liquid system

z_c	critical compressibility of i'th component
θ	Crank-Nicholson parameter (= 0 for fully explicit, = 1 for fully implicit)
ϕ	rock porosity
n	number of x-direction columns in system
Φ	flow potential term (except in reference to convergence pressure)
ρ_i	density at standard conditions of i'th component
λ	interblock mobility term for each phase
μ_i	low pressure, pure gas viscosity
τ	dummy factor in viscosity correlations
μ_m	low pressure gas mixture viscosity
μ	phase viscosity

Subscripts

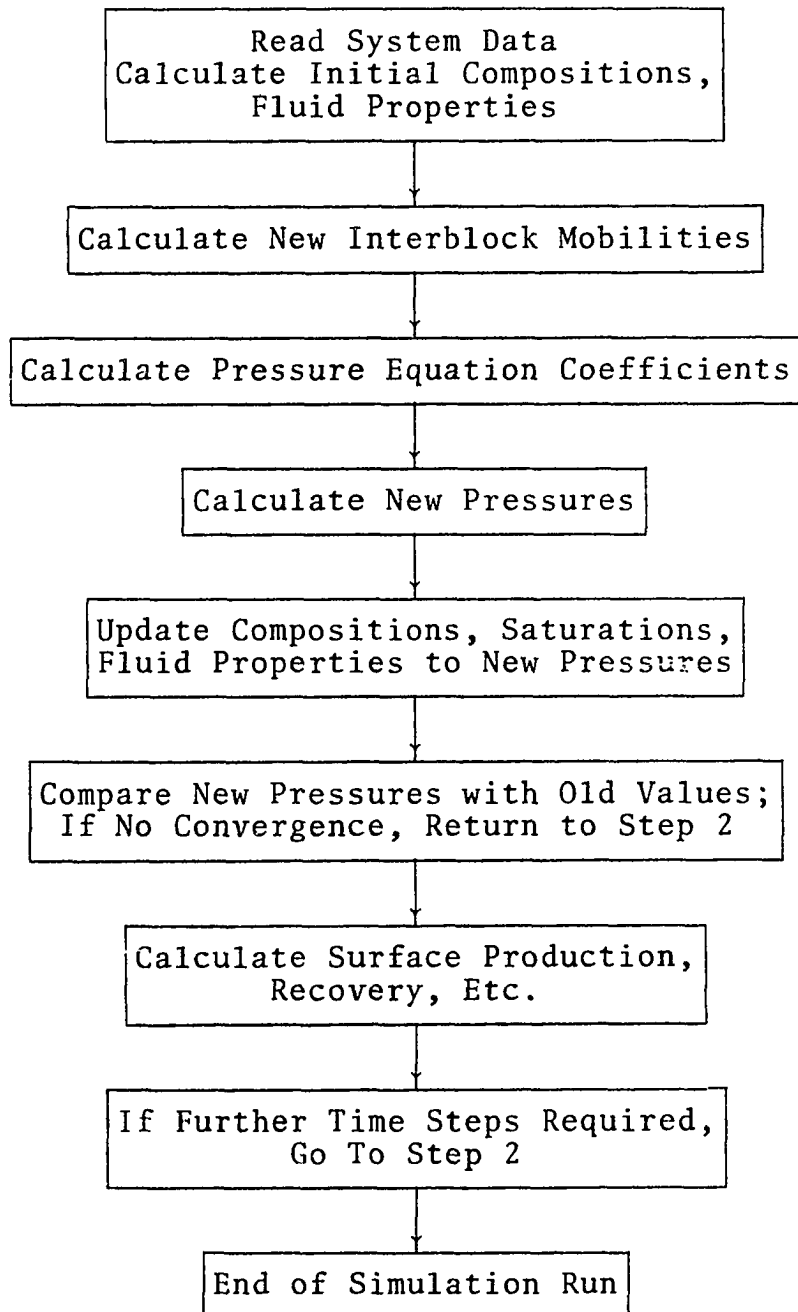
i	component or cell identifier
j	phase identifier (oil, gas, or water)
k	iteration counter
L	value for liquid phase
m	mixture value
V	value for vapor phase
$C7+$	value for heptanes-plus fraction

APPENDIX B

Flow Chart of Simulator

The simplified flow chart for the simulation package developed is presented on the following page.

Simplified Compositional Simulator Flow Chart

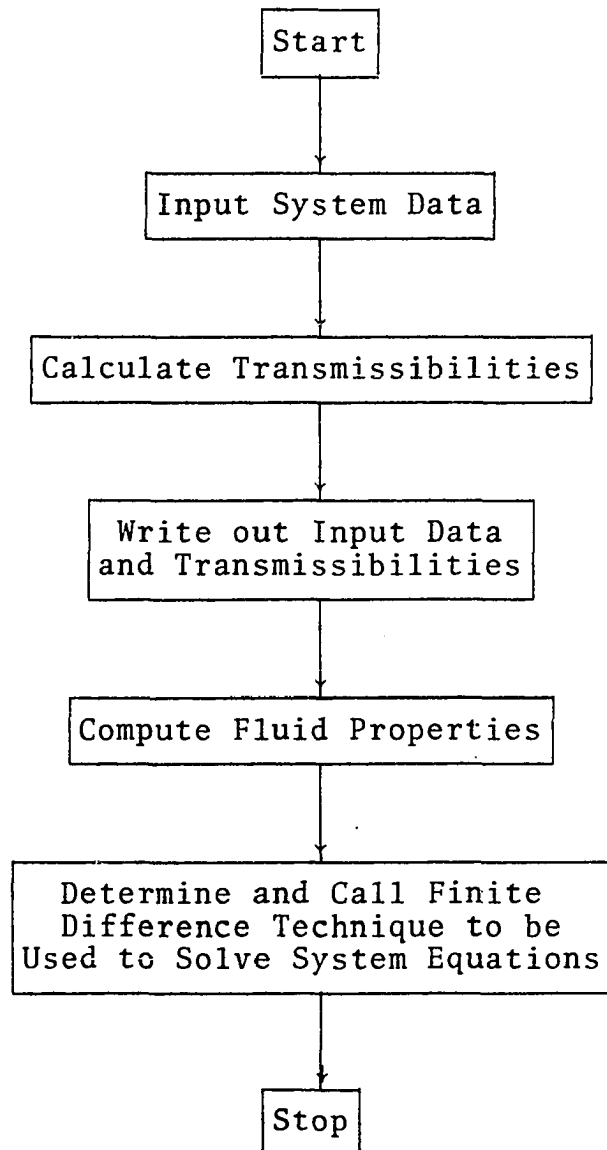


APPENDIX C

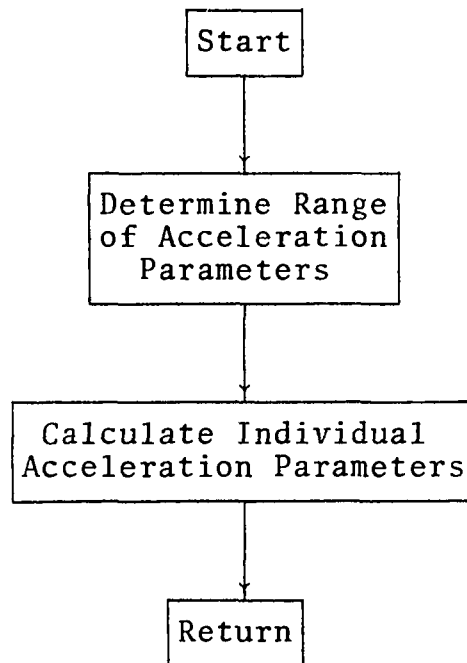
Flow Charts of Individual Subroutines

Flow charts of each of the subroutines used in this reservoir simulation package are presented on the following pages.

Flow Chart for Mainline



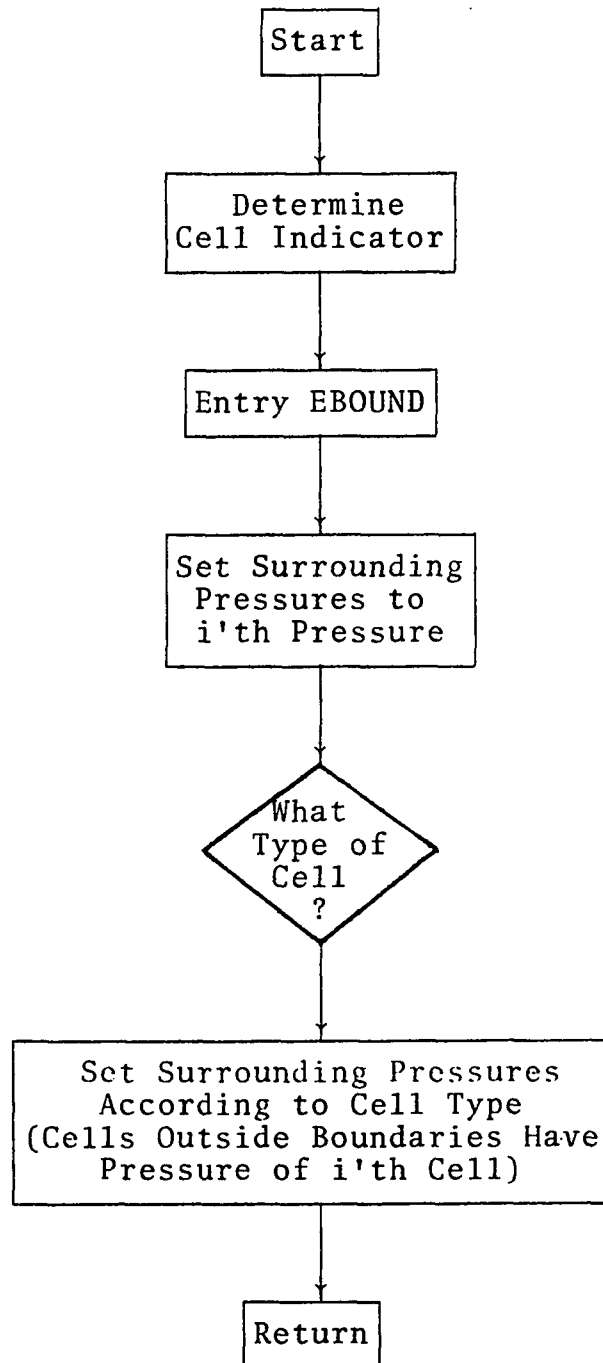
Flow Chart for Subroutine ACCP



Purpose of Subroutine:

To determine the acceleration parameter values to be used in the Iterative Alternating Direction Procedure when none are specified by the package user.

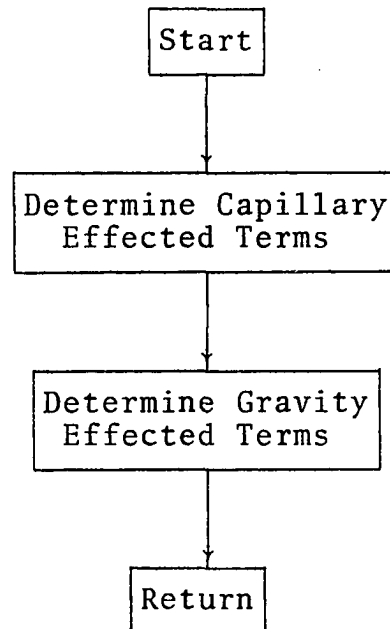
Flow Chart for Subroutine BOUND



Purpose of Subroutine:

To determine values to be used for surrounding cells based on their position in the model.

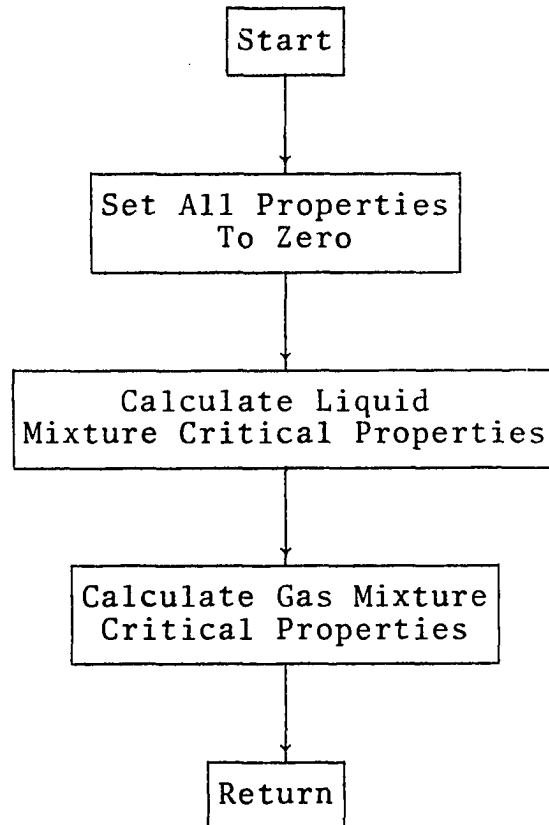
Flow Chart for Subroutine CPGRV



Purpose of Subroutine:

To determine the values of the capillary and gravity terms of the finite difference equations.

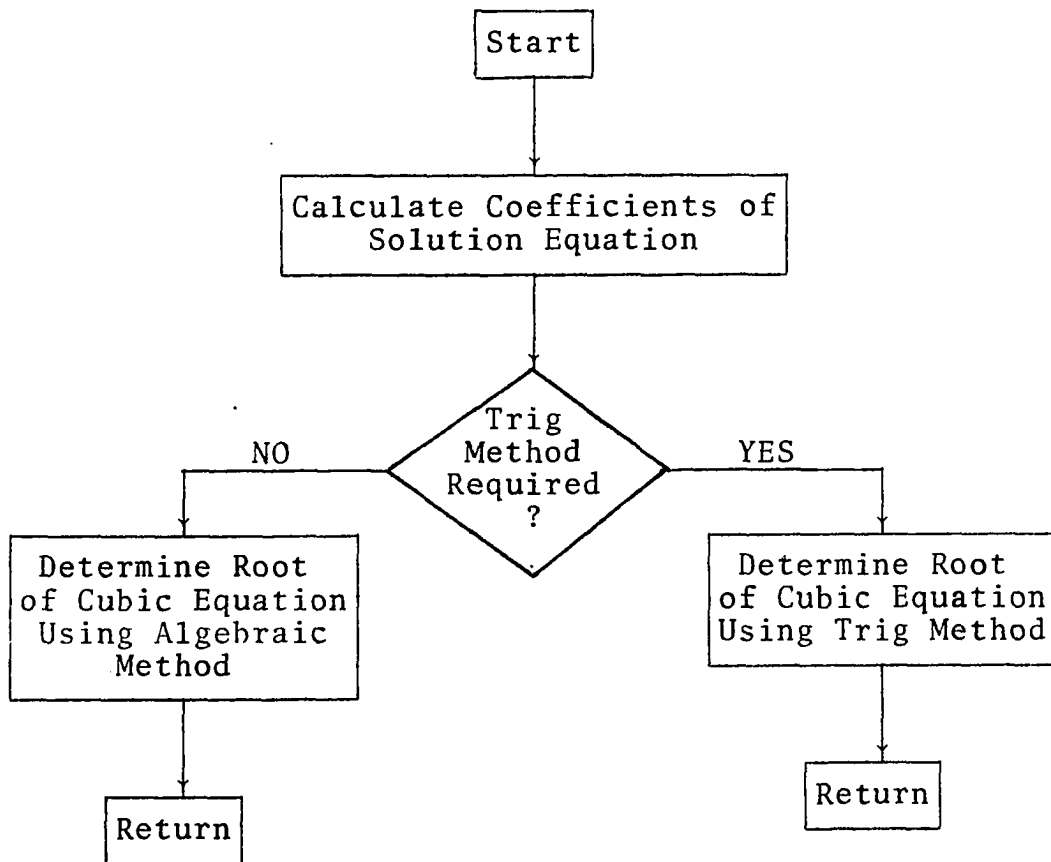
Flow Chart for Subroutine CRTPRP



Purpose of Subroutine:

To determine the liquid and vapor critical properties for a given hydrocarbon system.

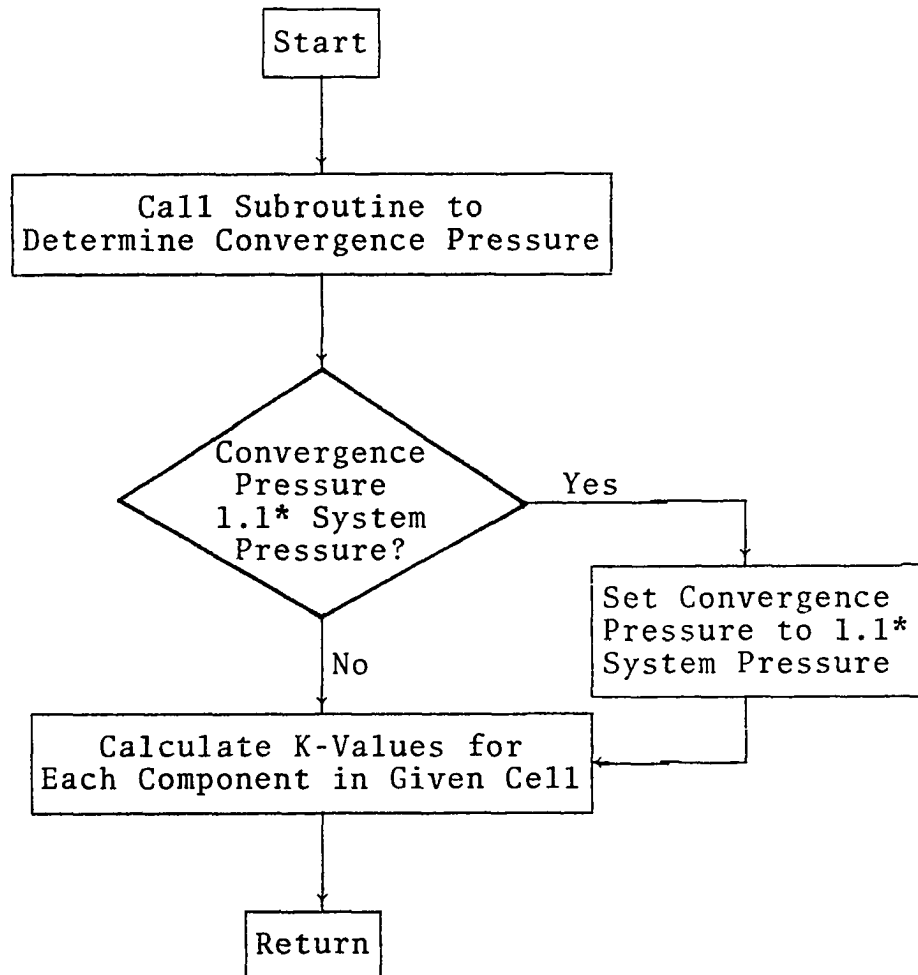
Flow Chart for Function CUBEQN



Purpose of Subroutine:

To determine the smallest positive root of a cubic equation.

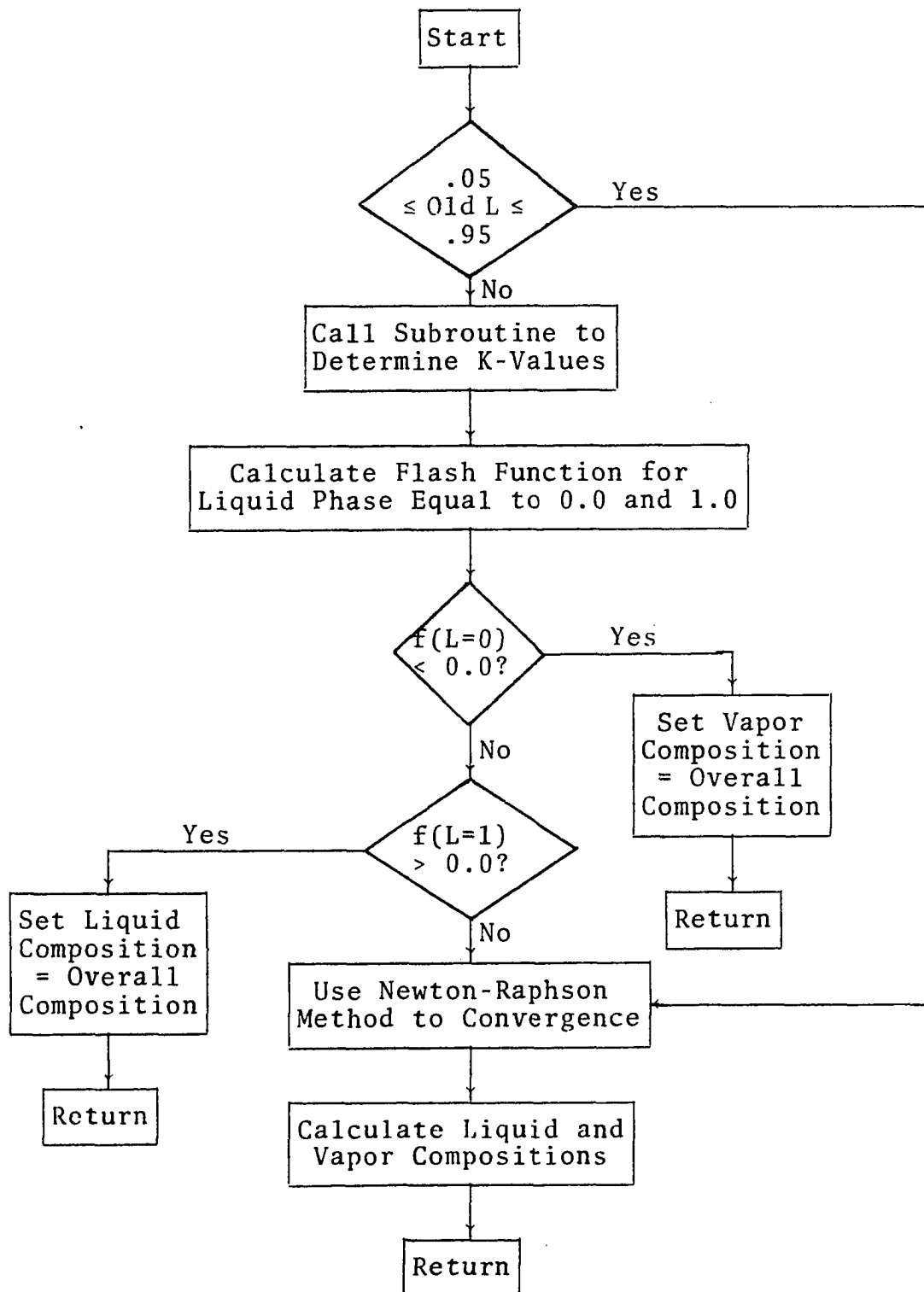
Flow Chart for Subroutine EQUILK



Purpose of Subroutine:

To determine the equilibrium K-Values for a given system.

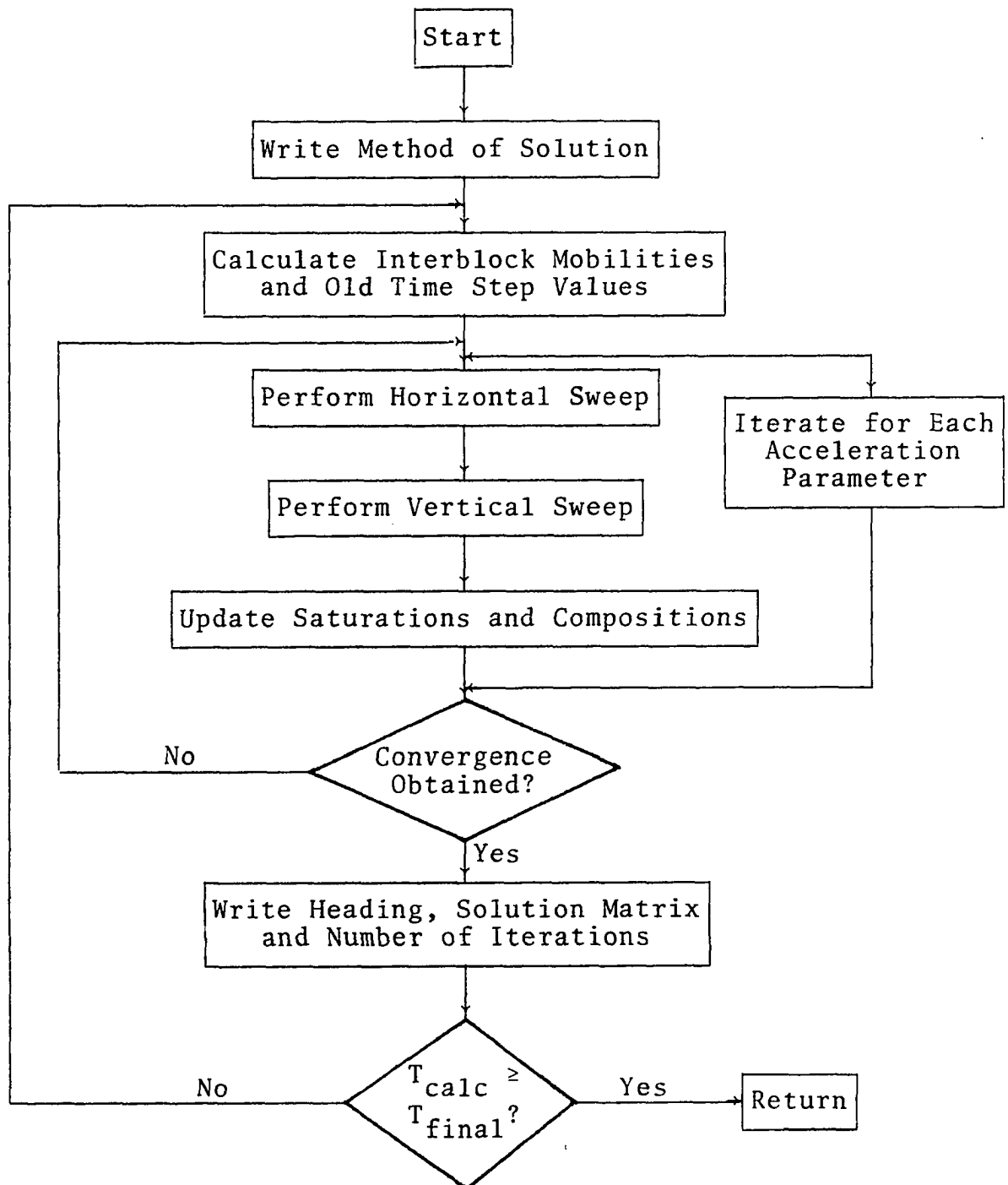
Flow Chart for Subroutine FLASH



Purpose of Subroutine:

To perform a flash calculation on a given fluid system.

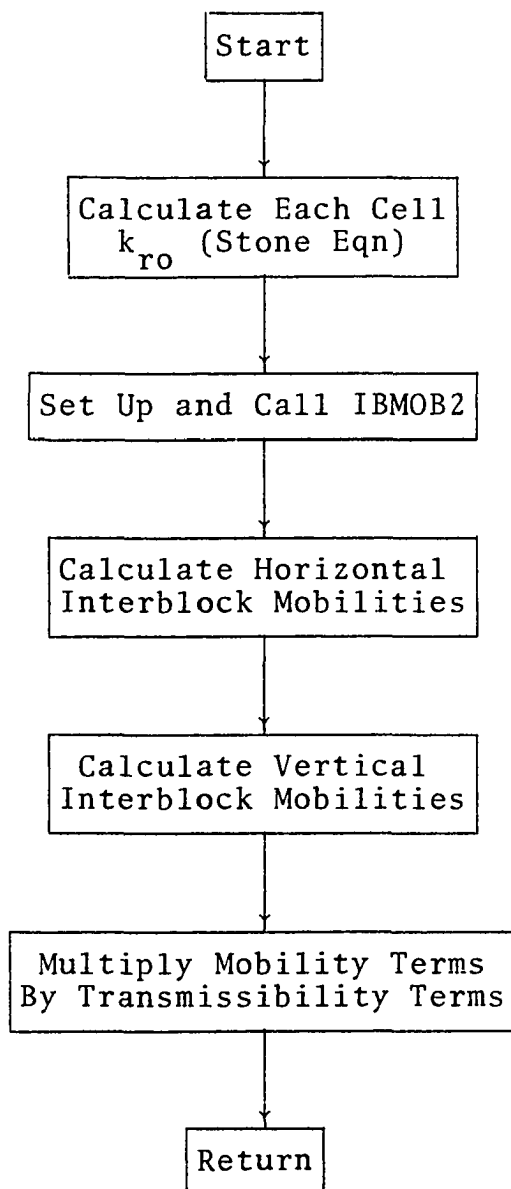
Flow Chart for Subroutine IADIP



Purpose of Subroutine:

To perform the iterative or non-iterative Alternating Direction Implicit Procedure on a given grid system.

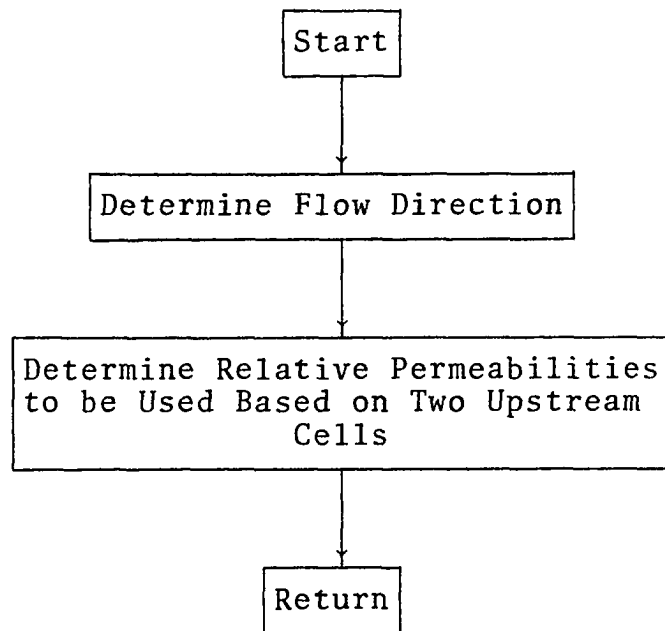
Flow Chart for Subroutine IBMOB1



Purpose of Subroutine:

To determine the interblock mobility terms for a given system.

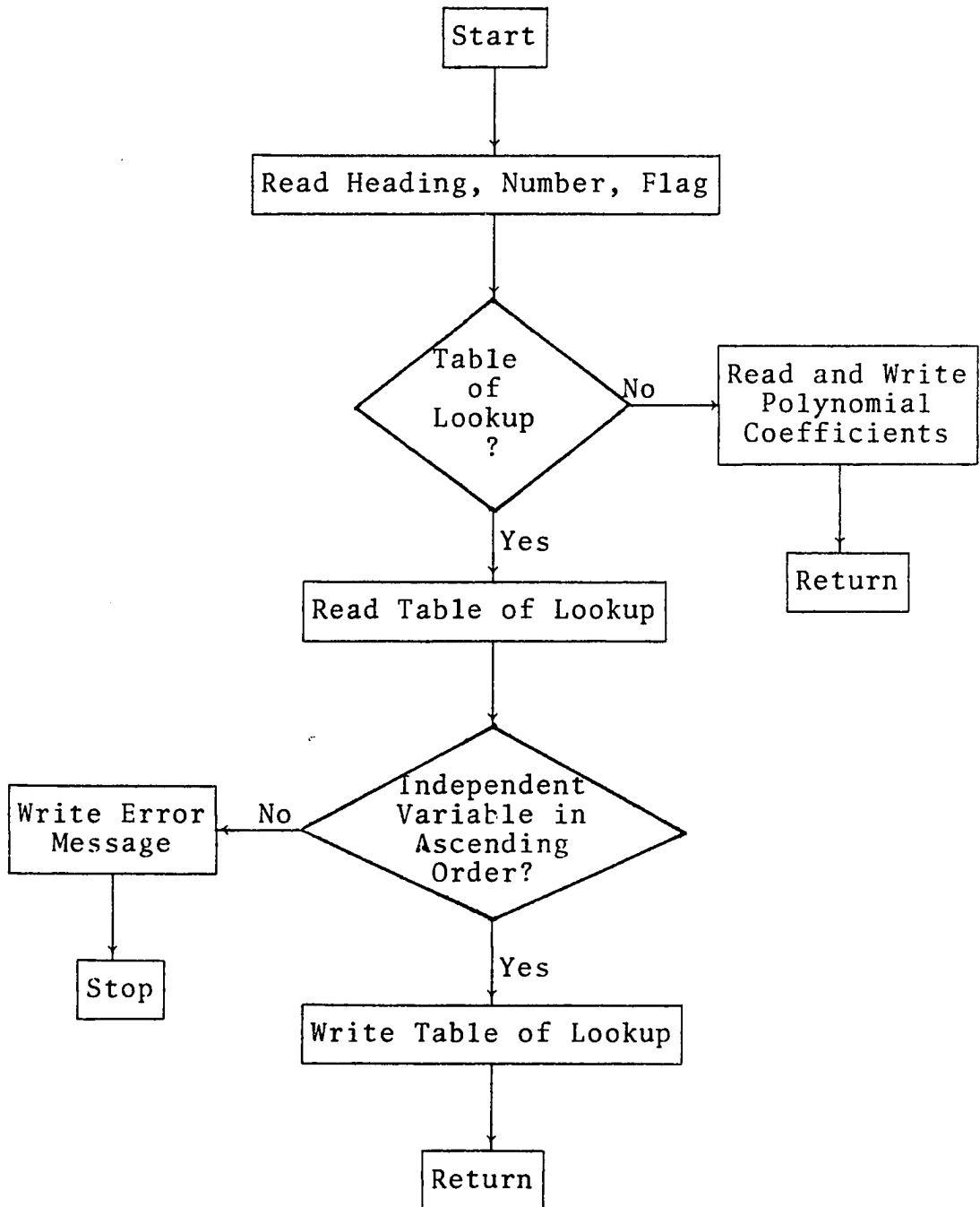
Flow Chart for Subroutine IBMOB2



Purpose of Subroutine:

To supplement IBMOB1 in determining the interblock mobilities.

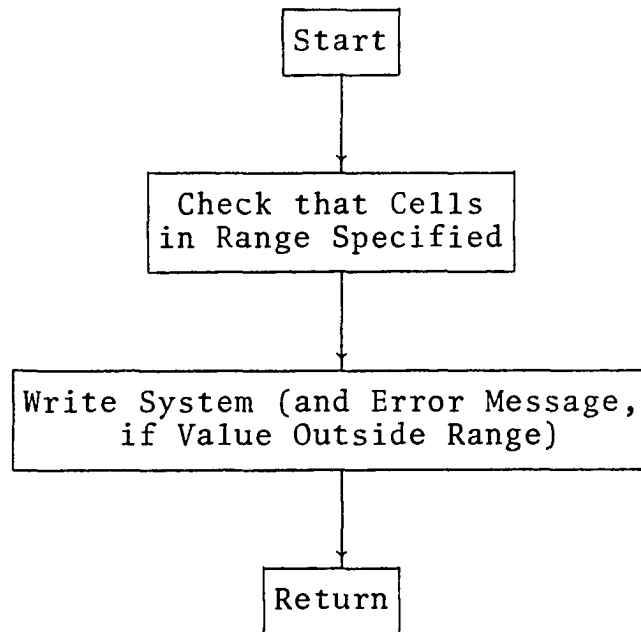
Flow Chart for Subroutine INDATA



Purpose of Subroutine:

To read in data as a table of lookup or polynomial coefficients.

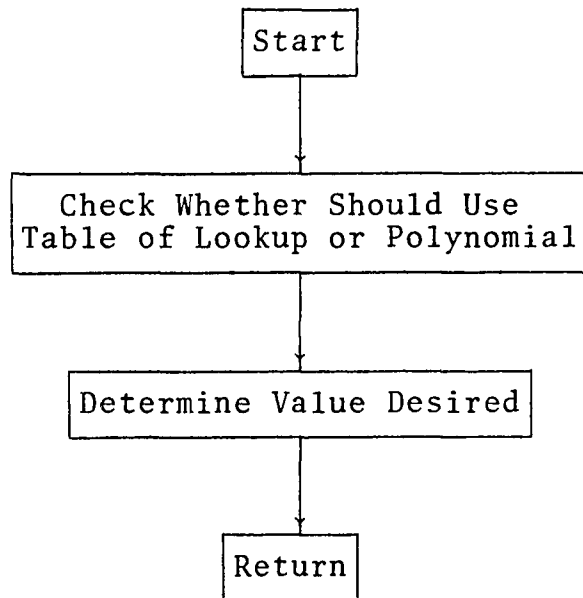
Flow Chart for Subroutine INPUT



Purpose of Subroutine:

To read data matrices, assigning a value to each cell, and check that data lie within range specified.

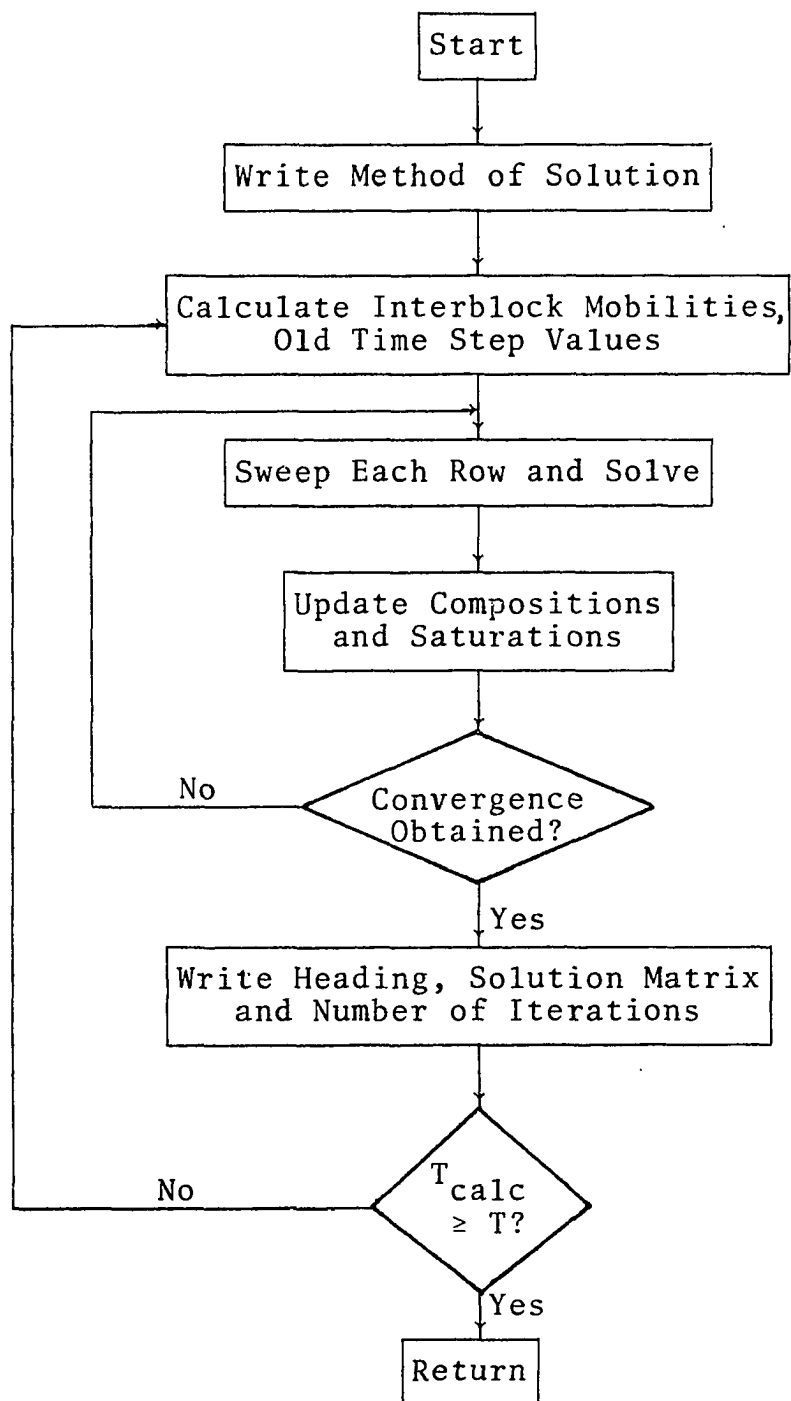
Flow Chart for Subroutine LOOKUP



Purpose of Subroutine:

To use table of lookup data or polynomial curve fit data to determine dependent value from given independent value.

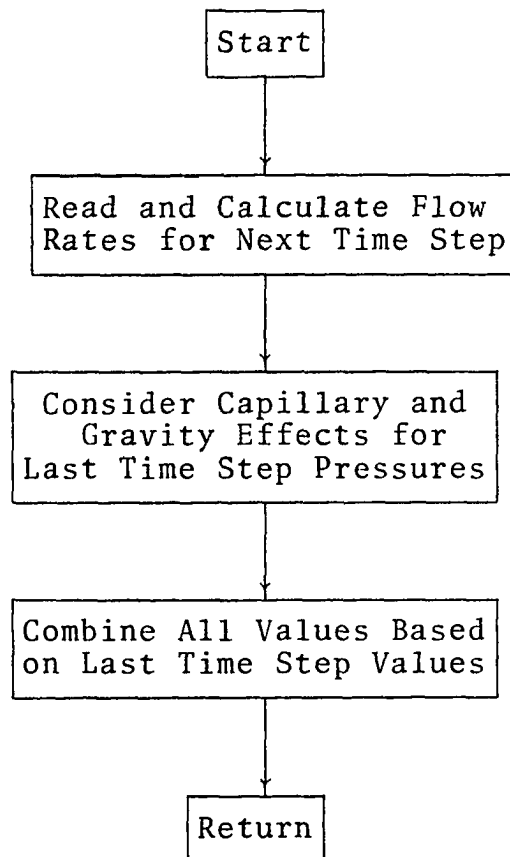
Flow Chart for Subroutine LSOR



Purpose of Subroutine:

To perform the Line Successive Over-Relaxation Procedure on a given system.

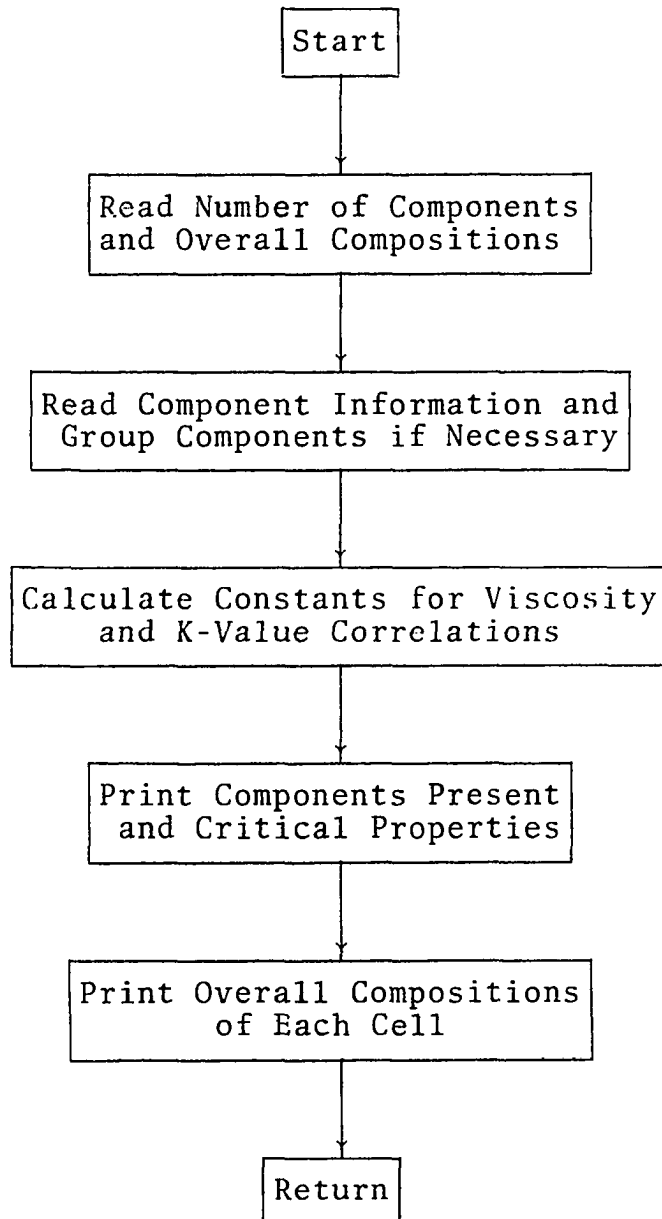
Flow Chart for Subroutine OLDT



Purpose of Subroutine:

To calculate all values based on values from last time step.

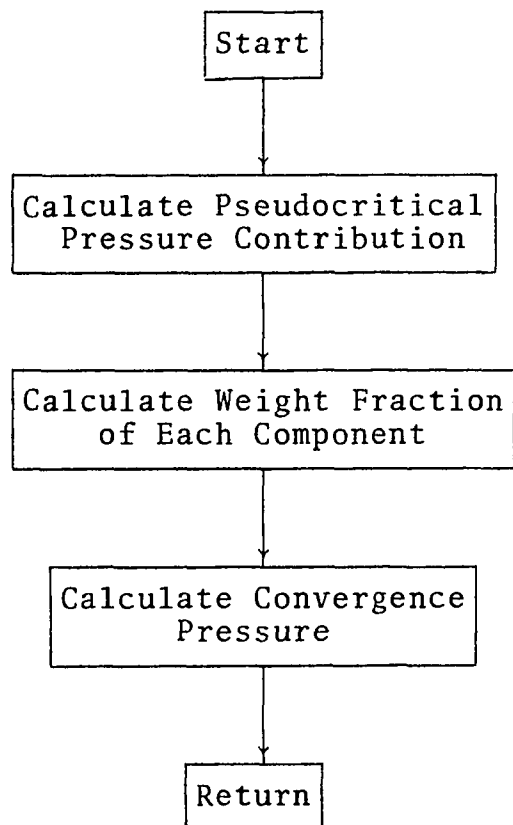
Flow Chart for Subroutine ONCE



Purpose of Subroutine:

To read component data and perform all of the one-time calculations for fluid properties.

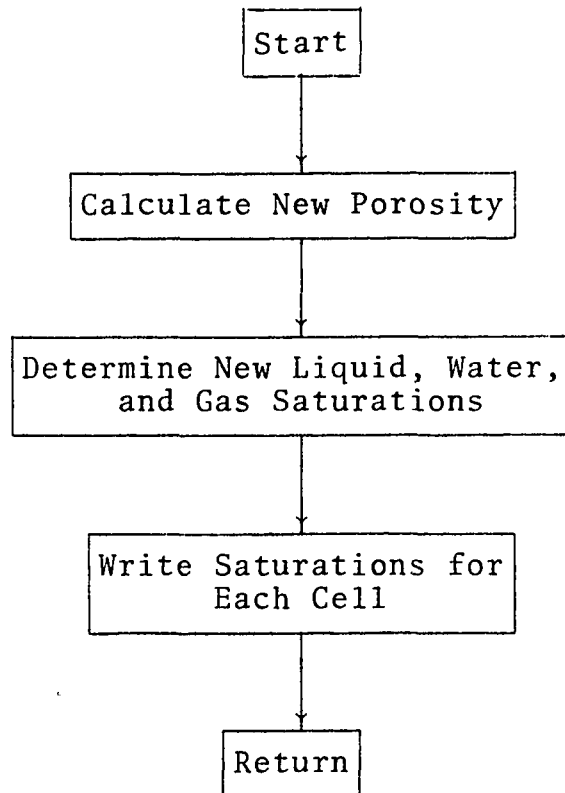
Flow Chart for Subroutine PCONV



Purpose of Subroutine:

To determine the convergence pressure for a given system.

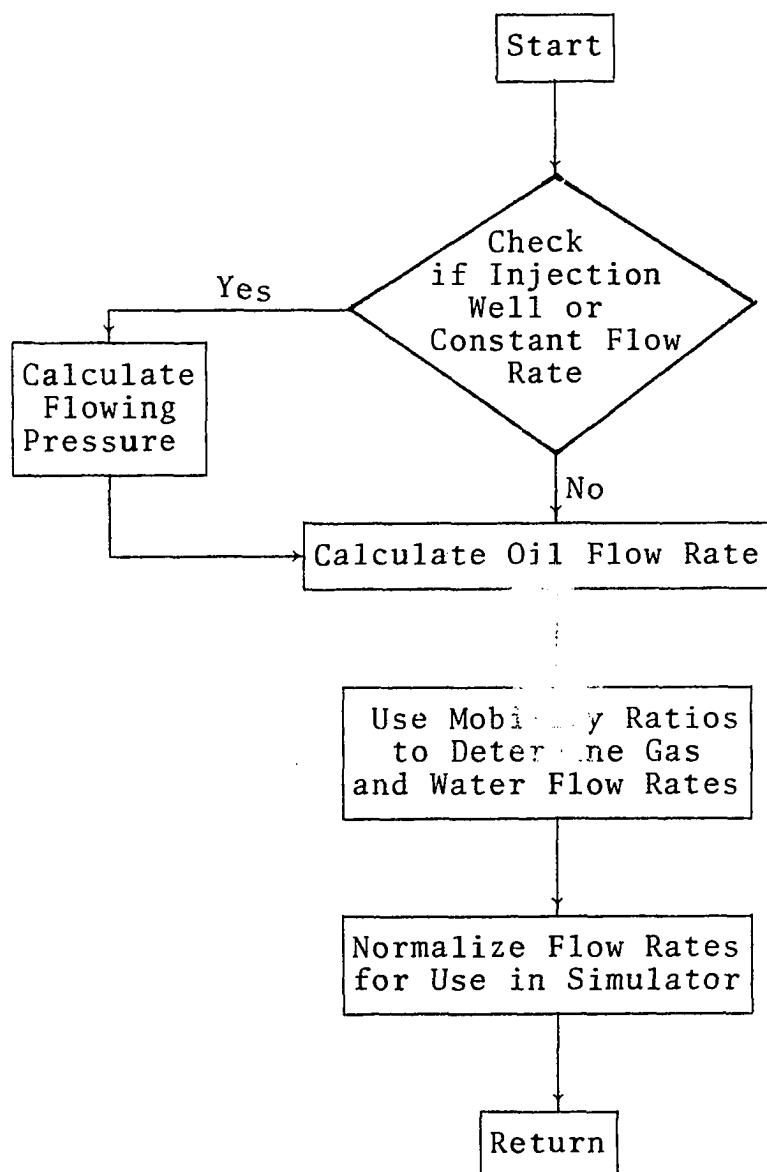
Flow Chart for Subroutine SATRN



Purpose of Subroutine:

To determine the liquid, gas, and water saturations for each cell of system.

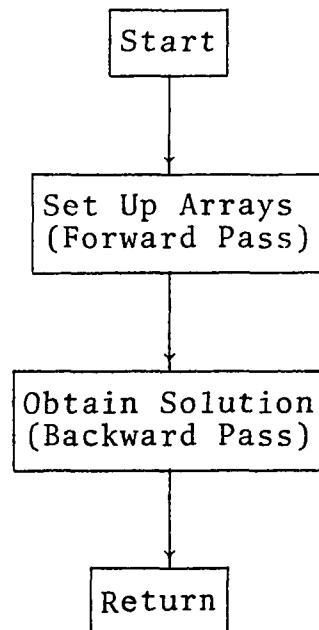
Flow Chart for Subroutine SORSNK



Purpose of Subroutine:

To calculate flow rates and flowing pressures for injector and producer cells.

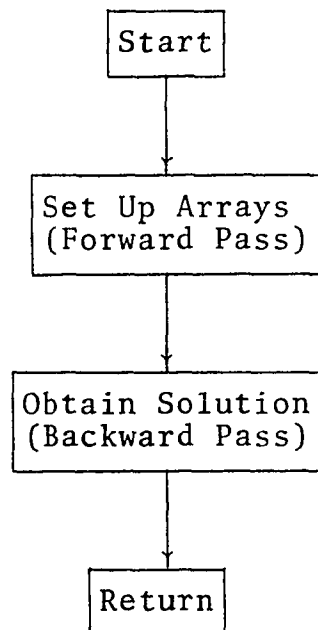
Flow Chart for Subroutine TRIHOR



Purpose of Subroutine:

To perform the horizontal version of the Thomas Algorithm for a close band tridiagonal matrix.

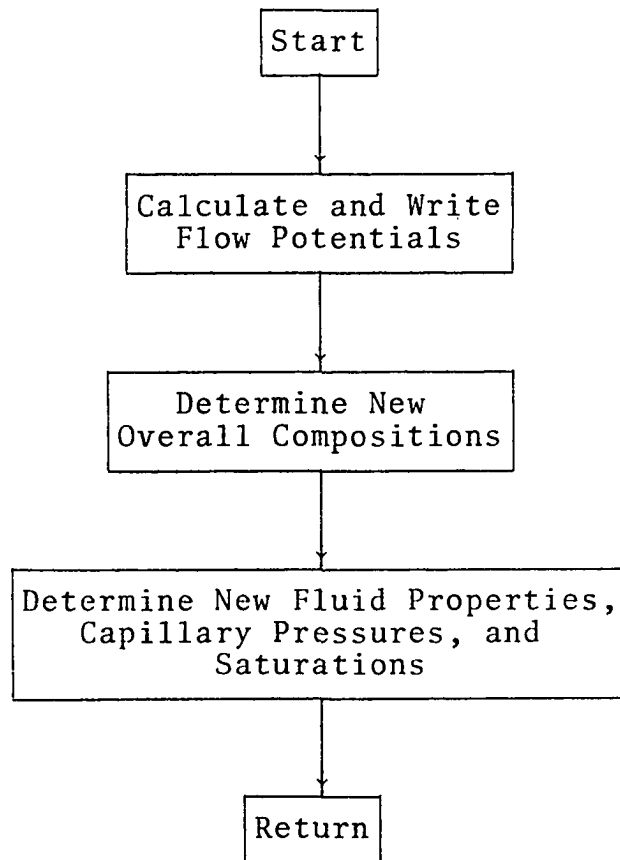
Flow Chart for Subroutine TRIVRT



Purpose of Subroutine:

To perform the vertical version of the Thomas Algorithm for a wide band tridiagonal matrix.

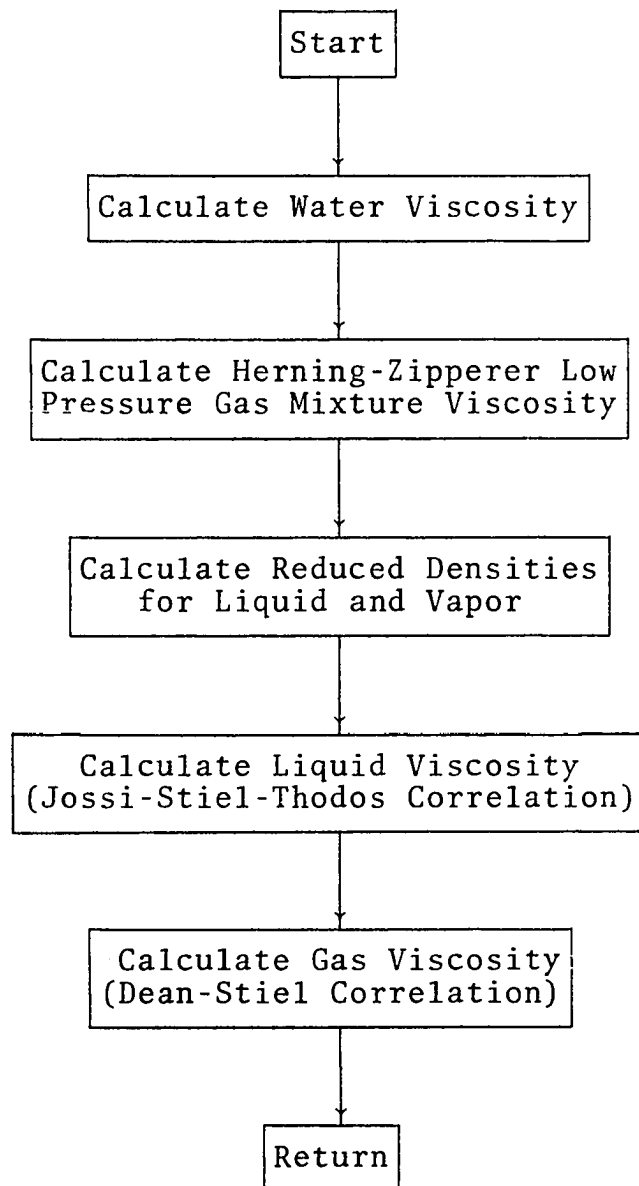
Flow Chart for Subroutine UPDATE



Purpose of Subroutine:

To update all values to the new pressure levels.

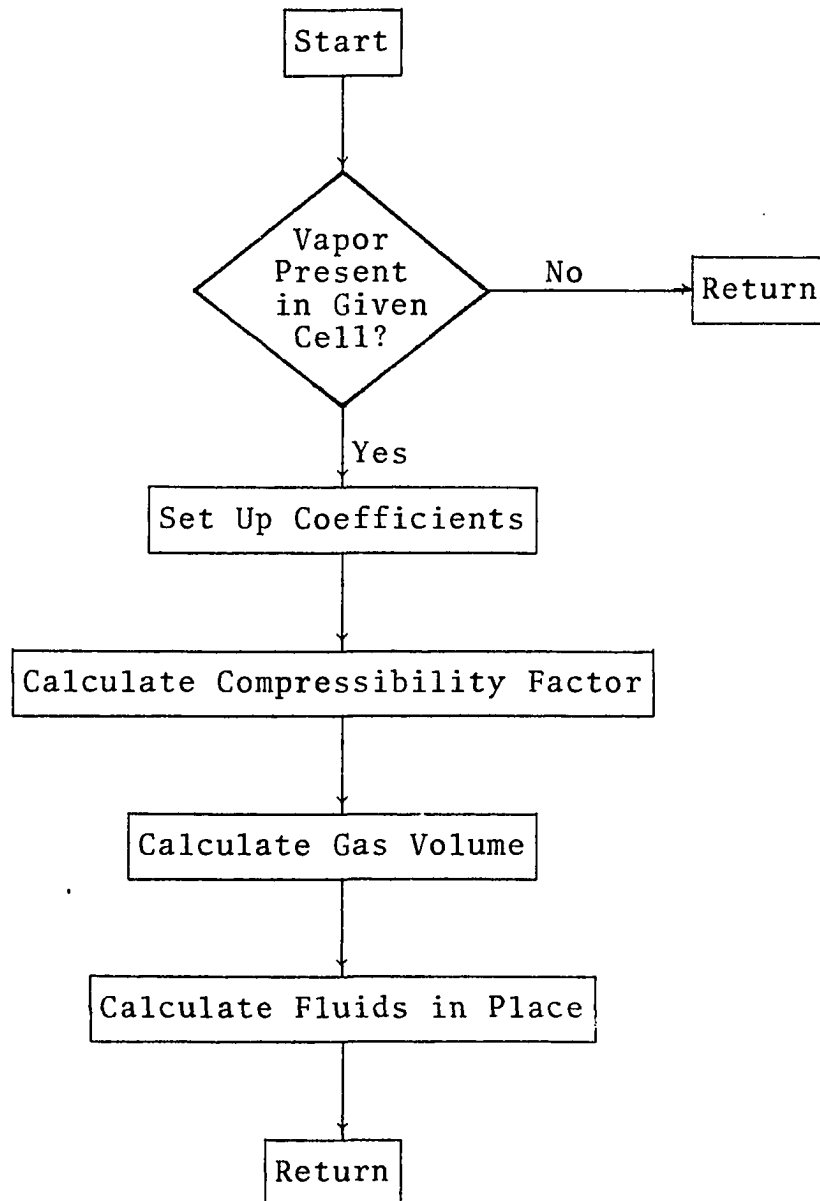
Flow Chart for Subroutine VISCTY



Purpose of Subroutine:

To determine each of the phase viscosities for a given system.

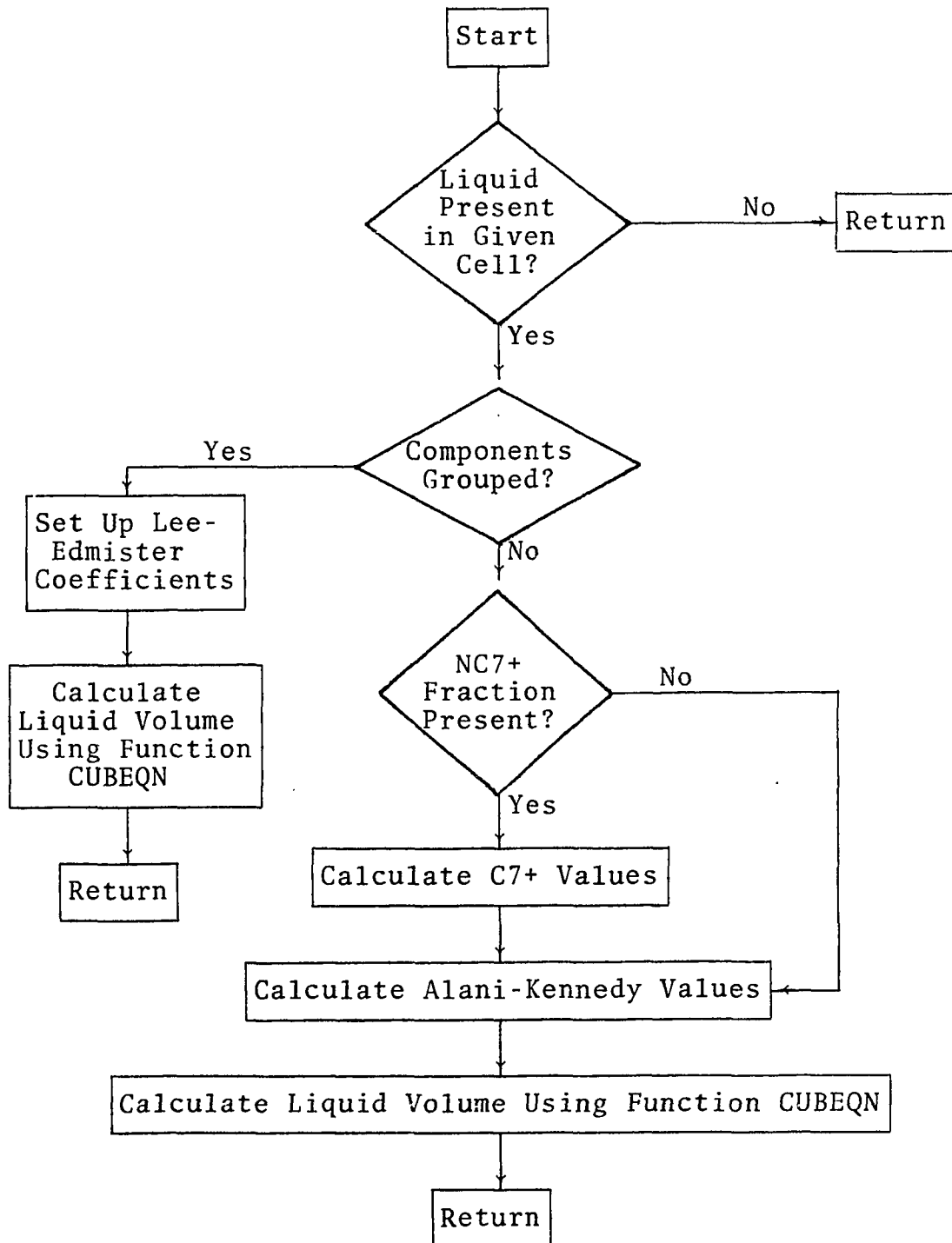
Flow Chart for Subroutine VOLGAS



Purpose of Subroutine:

To determine the vapor volume for a given system.

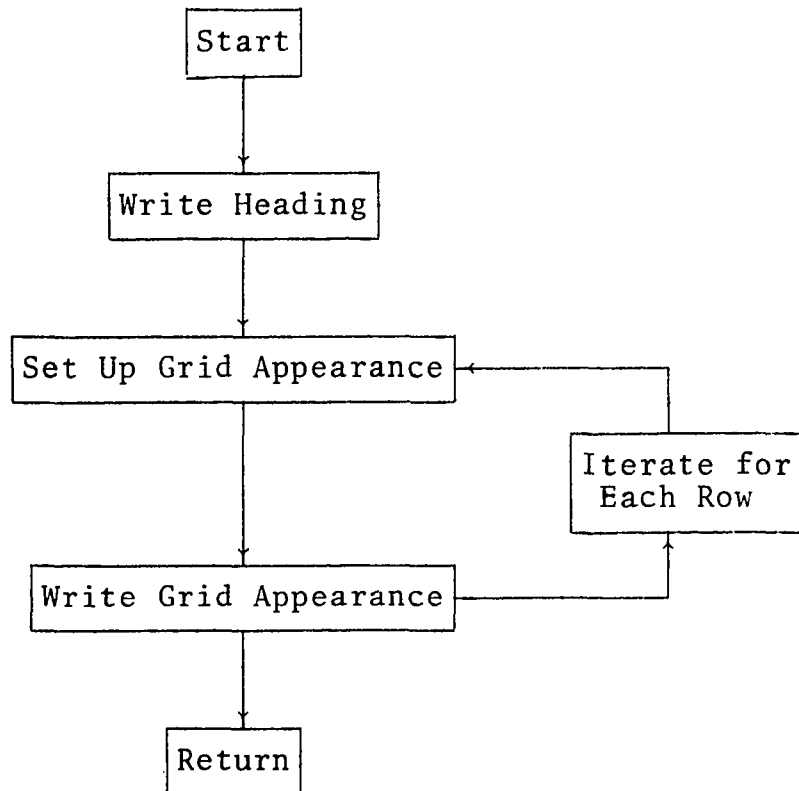
Flow Chart for Subroutine VOLLIQ



Purpose of Subroutine:

To determine the liquid volume for a given system.

Flow Chart for Subroutine WRTMOD



Purpose of Subroutine:

To output a representation of the grid system under consideration.

APPENDIX D

FORTRAN Listings

The FORTRAN listing for the simulation package developed is presented on the following pages.

C	THIS PROGRAM CANNOT BE RUN CONSECUTIVELY FOR SEVERAL DIFFERENT	00000010
C	SYSTEM CONFIGURATIONS; DEAD CELL VALUES MUST BE REZEROED FOR	00000020
C	DIFFERENT CONFIGURATIONS.	00000030
C		00000040
C		00000050
	BLOCK DATA	00000060
C	PURPOSE OF SUBPROGRAM:	00000070
C	TO INITIALIZE VARIOUS VALUES FOR USE IN THE SIMULATOR	00000080
	COMMON/IBMBTX/TLAMOX(500),TLAMGX(500),TLAMWX(500)	00000090
	COMMON/IBMBTY/TLAMOY(500),TLAMGY(500),TLAMWY(500)	00000100
	COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GH(500)	00000110
	COMMON/TRIDAG/A(500),B(500),C(500),D(500),IFRST,ILAST	00000120
	COMMON/RPERM/TKRO(500),TKRW(500),TKRG(500)	00000130
	COMMON/VSC TY/UMD(500),UMG(500),UMW(500)	00000140
	COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCELLS,NETA,NROW	00000150
	COMMON/PROD/QQ(50),QW(50),QG(50),NPQ(50),NQ	00000160
	COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)	00000170
	COMMON/INOUT/IN,IO,NFIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP	00000180
	COMMON/DNSTY/DL(500),DW(500),DG(500)	00000190
	COMMON/SATN/SW(500),SG(500),SQ(500),CF	00000200
	COMMON/TKH/TKHX(500),TKHY(500)	00000210
	COMMON/CPLRY/PCWO(500),PCGO(500),B1(500)	00000220
	DATA IN,IO/5,6/	00000230
	DATA GH,VOL,B,TKRO,UMD,UMG,UMW/3500*0.0/	00000240
	DATA TLAMOX,TLAMOY,TLAMGX,TLAMGY,TLAMWX,TLAMWY/3000*0.0/	00000250
	DATA DL,DG,DW,XL,ICN,NPQ/1560*0.0,80*0/	00000260
	DATA TKHX,TKHY,PCWO,PCGO,SQ,SG,SW/3500*0.0/	00000270
	END	00000280
C		00000290
C		00000300
C	PURPOSE OF MAINLINE:	00000310
C	TO INPUT ALL OF THE DATA REQUIRED TO DEFINE THE GRID	00000320
C	SYSTEM AND TO PERFORM SOME OF THE ONE TIME CALCULATIONS	00000330
	COMMON/FDIFF/DT,EPS,H(20),TF,THETA,ICT(250),NAP	00000340
	COMMON/CPLRY/PCWG(500),PCGC(500),B1(500)	00000350
	COMMON/DNSTY/DL(500),DW(500),DG(500)	00000360
	COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCELLS,NETA,NROW	00000370
	COMMON/TRIDAG/A(500),B(500),C(500),D(500),IFRST,ILAST	00000380
	COMMON/TKH/TKHX(500),TKHY(500)	00000390
	COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GH(500)	00000400
	COMMON/SATN/SW(500),SG(500),SQ(500),CF	00000410
	COMMON/FLUID3/AKROG(10),AKRCW(10),AKRG(10),AKRW(10)	00000420
	COMMON/FLUID4/SKROG(10),SKROW(10),SKRG(10),SKRW(10)	00000430
	COMMON/PERMF/NKROG,IFKROG,NKROW,IFKROW,NKRG,IFKRG,NKRW,IFKRW	00000440
	COMMON/IBMBTX/TLAMOX(500),TLAMGX(500),TLAMWX(500)	00000450

	COMMON/IBMBTY/TLAMOY(500),TLAMGY(500),TLAMWY(500)	00000460
	COMMON/RPERM/TKRO(500),TKRW(500),TKRG(500)	00000470
	COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)	00000480
	COMMON/INOUT/IN,IO,NFIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP	00000490
	COMMON/WTRV/AUW(10),PUW(10),NUW,IFUW	00000500
	COMMON/FVOLF/ABO(10),PBO(10),NBO,IFBO,ABW(10),PBW(10),NBW,IFBW	00000510
	COMMON/PCAPG/APCG(10),PPCG(10),NPCG,IFPCG	00000520
	COMMON/PCAPQ/APCQ(10),PPCQ(10),NPCQ,IFPCQ	00000530
	COMMON/COMP1/ACO(10),ACW(10),ACG(10),PCO(10),PCW(10),PCG(10)	00000540
	COMMON/COMP2/NCQ,NCW,NCG,IFCQ,IFCW,IFCG	00000550
	DIMENSION LDD(500),AK(500)	00000560
	EQUIVALENCE (AK(1),TKHY(1)),(BW,DELX)	00000570
C	NTYPE = -1; CONSIDER GRAVITY EFFECTS	00000580
C	NTYPE = 1; CONSIDER CAPILLARY EFFECTS	00000590
C	NTYPE = 0; CONSIDER NEITHER	00000600
C	NTYPE = 2; CONSIDER BOTH	00000610
	READ(IN,1001) METHOD,NAP,NCELLS,NETA,NIC,IFRST,ILAST,NTYPE,NFIP,NL	00000620
	&MDA,NSAT,NPOT,NCOMP,NTKH,NPMTX,NPLKUP	00000630
	DT=-1.0	00000640
1001	FORMAT(20I4)	00000650
	NROW=NCELLS/NETA	00000660
	READ(IN,1002) DELX,DELY,CF	00000670
1002	FORMAT(8F10.0)	00000680
	IF(DELX.LE.0.0) GO TO 40	00000690
	DO 50 I=1,NETA	00000700
50	DX(I)=DELX	00000710
	DO 60 I=1,NROW	00000720
60	DY(I)=DELY	00000730
	GO TO 70	00000740
40	READ(IN,1002) (DX(I),I=1,NETA)	00000750
	READ(IN,1002) (DY(I),I=1,NROW)	00000760
70	READ(IN,1001) (ICN(I),I=1,NIC)	00000770
	CALL WRTMOD	00000780
	NF=(NCELLS+3)/4	00000790
	READ(IN,1004) (ICT(I),I=1,NF)	00000800
1004	FORMAT(8I8)	00000810
	CALL INPUT(D,NPMTX)	00000820
	CALL INPUT(AK,NPMTX)	00000830
	AKA=AK(IFRST)	00000840
	CALL INPUT(HT,NPMTX)	00000850
C	TRANSMISSIBILITY CALCULATION	00000860
	NF=IFRST+1	00000870
	KY=1+(IFRST-1)/NETA	00000880
	KX=IFRST-NETA*(KY-1)	00000890
	TKHX(IFRST)=AK(IFRST)*HT(IFRST)*DY(KY)/DX(KX)	00000900


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        TKHY(IFIRST)=AK(IFIRST)*HT(IFIRST)*DX(KX)/DY(KY)
DO 61 I=NF,1,LAST
  IF(HT(I).EQ.0.0) GO TO 61
  AKA=AKA+AK(I)
  KY=1+(I-1)/NETA
  KX=I-NET*AK(KY-1)
  TKHX(I)=AK(I)*HT(I)*DY(KY)/DX(KX)
  TKHY(I)=AK(I)*HT(I)*DX(KX)/DY(KY)
  IF(KX.EQ.1.0R,HT(I-1).EQ.0.0) GO TO 64
  TKHX(I-1)=(TKHX(I)+TKHX(I-1))/(DX(KX)+DX(KX-1))
  IF(I.LE.NETA.0R,HT(I-NETA).EQ.0.0) GO TO 61
  TKHY(I-NETA)=(TKHY(I)+TKHY(I-NETA))/(DY(KY)+DY(KY-1))
CONTINUE
AKA=AKA/(LAST-IFIRST-NIC+1)
IF(NIKH.EQ.0) GO TO 55
WRITE(IO,1008)
FORMAT('1TRANSMISSIBILITY MATRICES')
DO 56 I=NETA,NCELLS,NETA
  WRITE(IO,1007) (TKHX(I+J-NETA),J=1,NETA)
  FORMAT('X-DIR..2X,10E12.4')
  WRITE(IO,1011) (TKHY(I+J-NETA),J=1,NETA)
  FORMAT('Y-DIR..2X,10E12.4')
CONTINUE
IF(NTYPE.NE.-1.AND,NTYPE.NE.2) GO TO 53
DO 54 I=IFIRST,1,LAST
  C  SET UP GRAVITY * THICKNESS TERM AND CONVERT UNITS
54  GH(I)=.223611*HT(I)
53  CALL INPUT(PHI,NPMTX)
  CALL INPUT(SO,NPMTX)
  CALL INPUT(SG,NPMTX)
  CALL INPUT(SW,NPMTX)
  CALL INPUT(ZEL,NPMTX)
  CALL INPUT(LDD,NPMTX)
  IF(NPLKUP.NE.0) WRITE(IO,1003)
1003 FORMAT('1.')
  CALL INDATA(AUW,PUM,NUW,IFUW)
  CALL INDATA(ABD,PBD,NBD,IFBD)
  CALL INDATA(ABW,PBW,NBW,IFBW)
  CALL INDATA(AKROG,SKROG,NKROG,IFKROG)
  CALL INDATA(AKRG,SKRG,NKRG,IFKRG)
  CALL INDATA(AKRW,SKRW,NKRW,IFKRW)
  CALL INDATA(APCO,PPCO,NPCO,IFPCO)
  CALL INDATA(APCG,PPCG,NPCG,IFPCG)
  CALL INDATA(ACD,PCD,NCD,IFCC)

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      CALL INDATA(ACW,PCW,NCW,IFCW)
      CALL INDATA(ACG,PCG,NCG,IFCG)
      READ(IN,1002) PWC,PGOC,ZOWC,ZGOC
      READ(IN,1002) (H(I),I=1,NAP)
      C THETA = 0, EXPLICIT; THETA = 1, IMPLICIT
      READ(IN,1002) TF,THETA,EPS,T
      CALL ONCE
      WRITE(10,1006) CF,THETA,EPS,T,TF
1006  FORMAT('ROCK COMP. FACTOR =',E13.6,'/',' THETA =',F7.4,'/',' CONVERGE
      GENCE TOLERANCE =',E10.3,'/',' SYSTEM TEMPERATURE IS',F6.1,' DEGREE
      S FARENHEIT',',',',', TIME SPAN TO BE SIMULATED IS',F7.1,' DAYS.')
      J=1
      DO 90 I=IFRST,ILAST
      IF(ICN(J).NE.I) GO TO 92
      J=J+1
      GO TO 90
92  NF=1+(I-1)/NETA
      VOL(I)=DX(I-NEA*(NF-1))*DY(NF)*HT(I)*PHI(I)
      NF=N*(I-1)
      CALL FLASH(D(I),NF,I)
      CALL CRTRP(D(I),NF,I)
      CALL LOOKUP(PCWD(I),SG(I),APCO,PPCO,NPCO,IFPCO)
      CALL LOOKUP(PCGD(I),SG(I),APCG,PPCG,NPCG,IFPCG)
      CALL LOOKUP(CO,D(I),ACD,PCD,NCOD,IFCO)
      CALL LOOKUP(CW,D(I),ACW,PCW,NCW,IFCW)
      CALL LOOKUP(CG,D(I),ACG,PCG,NCG,IFCG)
      B1(I)=CF+SD(I)*CO+SW(I)*CW+SG(I)*CG
90  CONTINUE
      IF(D(IFRST).NE.0.0) GO TO 51
      DO 52 I=IFRST,ILAST
      C FIND INITIAL PRESSURE FROM WATER-OIL CONTACT PRESSURE MINUS DENSITY*
      C GRAVITY*THICKNESS
52  D(I)=PWC-DL(I)*.2236111*ZEL(I)
      WRITE(10,1009)
1009  FORMAT('ESTIMATED INITIAL PRESSURE BASED ON DENSITY, FORMATION EL
      EVATION, AND WATER-OIL CONTACT')
      DO 58 I=NETA,NCELS,NETA
      WRITE(10,1010) (D(I+J-NETA),J=1,NETA)
1010  FORMAT('/',10F10.0)
58  CONTINUE
59  IF(METHOD.EQ.2) GO TO 81
80  CALL IADIP(AKA,NTYPE)
      STOP
81  CALL LSOR(NTYPE)

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1005 WRITE(10,1005) DY(J/NETA), (NPQ(I), NC(I), NPQ(I+2*NETA), I=1, NETA)
      FORMAT(3X, F7.1, 8(., /), ., +., ., 11(A2, I3, I1X, A3))
1006 WRITE(10,1006) (NB1, I=1, M), (NS1, I=1, 8)
      FORMAT(., +., ., 17X, 100A1)
10   WRITE(10,1004) ((NPQ(I+(L-1)*NETA), L=1, 3), I=1, NETA), NS2, NS4, NS2B
      CONTINUE
      WRITE(10,1002) (NP1, I=1, M), (NS1, I=1, 8)
      DO 60 KK=1, 4
        WRITE(10,1002) (NS1, I=1, M), (NS1, I=1, 8)
        CONTINUE
      RETURN
      END

C
C
C   SUBROUTINE INPUT(E, NPMTX)
C   PURPOSE OF SUBROUTINE:
C   TO READ DATA MATRICES, ASSIGNING A VALUE TO EACH CELL OF SYSTEM
C   AND CHECK THAT IT LIES WITHIN THE RANGE SPECIFIED FOR THE DATA
COMMON/SYSTEM/DX(20), DY(20), ICN(30), METHOD, NIC, NCELLS, NETA, NROW
COMMON/TRIDAG/A(500), B(500), C(500), D(500), IFRST, ILAST
COMMON/INOUT/IN, IO, NFIP, NLMDA, NSAT, NPOT, NCOMP, NTKH, NPLKUP
DIMENSION E(NCELLS), NX(10)
READ(IN, 1001) (NX(I), I=1, 10), FACTOR, XMIN, XMAX
FORMAT(10A4, 4F10.0)
1001 IF(NPMTX.NE.0) WRITE(10,1002) (NX(I), I=1, 10), FACTOR, XMIN, XMAX
1002 FORMAT(., 1., 5X, 10A4, 5X, ., FACTOR = ., F9.4, 5X, ., MIN VALUE = ., F9.4, 5X,
      E, MAX VALUE = ., F9.4, ., /)
      IF(IFRST.EQ.1) GO TO 61
      J1=IFRST-1
      DO 64 I=1, J1
        E(I)=0.0
        IF(ILAST.EQ.NCELLS) GO TO 62
        J1=ILAST+1
        DO 63 I=J1, NCELLS
          E(I)=0.0
          IF(XMAX.LE.XMIN) GO TO 40
          DO 10 I=NETA, NCELLS, NETA
            READ(IN, 1003) (E(J+I-NETA), J=1, NETA)
            FORMAT(8F10.0)
            IF(NPMTX.NE.0) WRITE(10,1004) (E(J+I-NETA), J=1, NETA)
            FORMAT(/, 11F11.4)
          CONTINUE
          J1=I
          DO 20 I=IFRST, ILAST
            IF(E(I).GT.XMAX) GO TO 31
1003
1004
10

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IF(E(I).GE.XMIN) GO TO 21	00002710
J2=J1	00002720
DO 30 J=J2,NIC	00002730
IF(I.NE.ICN(J)) GO TO 30	00002740
J1=J	00002750
E(I)=0.0	00002760
GO TO 20	00002770
30 CONTINUE	00002780
31 WRITE(IO,1005) I	00002790
1005 FORMAT(//,' CELL NUMBER',I4,' OF THE ABOVE MATRIX IS OUTSIDE THE BOUNDS SPECIFIED FOR THE DATA.',//,10X,'EXECUTION TERMINATING')	00002800
NX(1)=-1	00002810
21 E(I)=E(I)*FACTOR	00002820
20 CONTINUE	00002830
IF(NX(1).LT.0) STOP	00002840
RETURN	00002850
40 DO 50 I=IFRST,ILAST	00002860
50 E(I)=XMIN	00002870
DO 51 I=1,NIC	00002880
51 E(ICN(I))=0.0	00002890
DO 60 I=NETA,NCCELLS,NETA	00002900
IF(NPMTX.NE.0) WRITE(IO,1004) (E(J+I-NETA),J=1,NETA)	00002910
60 CONTINUE	00002920
RETURN	00002930
END	00002940
C	00002950
C	00002960
SUBROUTINE INDATA(A,P,KN,IFLAG)	00002970
C PURPOSE OF SUBROUTINE:	00002980
C TO READ IN DATA AS TABLE OF LOOKUP OR POLYNOMIAL COEFFICIENTS	00002990
COMMON/INOUT/IN,IO,NFIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP	00003000
DIMENSION A(10),P(10),NX(10)	00003010
READ(IN,1001) (NX(I),I=1,10),KN,IFLAG	00003020
1001 FORMAT(10A4,2I5)	00003030
IF(IFLAG.GT.1) GO TO 10	00003040
C READ POLYNOMIAL COEFFICIENTS	00003050
READ(IN,1002) (A(I),I=1,KN)	00003060
1002 FORMAT(6F13.0)	00003070
IF(NPLKUP.NE.0) WRITE(IO,1003) (NX(I),I=1,10),(A(I),I=1,KN)	00003080
1003 FORMAT(///,' POLYNOMIAL COEFFICIENTS FOR ',10A4,/,(/,E14.6))	00003090
RETURN	00003100
C READ TABLE OF LOOK-UP INFORMATION	00003110
10 PI=0.0	00003120
DO 20 I=1,KN	00003130
READ(IN,1004) P(I),A(I)	00003140
	00003150

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1004 FORMAT(2F10.0)
      IF(PI.GT.P(I)) IFLAG=10
20    PI=P(I)
1005 IF(NPLKUP.NE.0) WRITE(IO,1005) (NX(I),I=1,10),(P(I),A(I),I=1,KN)
      FORMAT(/,/, 'TABLE OF LOOK-UP INFORMATION FOR ',10A4,/,5X,'DEPENDEN
      ENT',5X,'INDEPENDENT',/,/(,2E16.6))
      IF(IFLAG.LE.9) RETURN
1006 WRITE(IO,1006) (NX(I),I=1,10)
      FORMAT(/,/, 'INDEPENDENT VARIABLES IN TABLE OF LOOK-UP FOR ',10A4,
      & ARE NOT IN ASCENDING ORDER.,/,10X,'EXECUTION TERMINATED.,')
      STOP
      END
C
C
C SUBROUTINE SORSNK(AKG,PWF,S,L,NIND)
C PURPOSE OF SUBROUTINE:
C TO DETERMINE THE FLOW AT A SOURCE OR A SINK GIVEN THE FLOWING
C BOTTOM HOLE PRESSURE
      COMMON/DNSTY/DL(500),DW(500),DG(500)
      COMMON/IBMBTX/TLAMOX(500),TLAMGX(500),TLAMWX(500)
      COMMON/IBMBTY/TLAMOY(500),TLAMGY(500),TLAMWY(500)
      COMMON/INOUT/IN,IO,NFIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP
      COMMON/VSC TY/UMO(500),UMG(500),UMW(500)
      COMMON/PROD/QO(500),QW(500),QG(500),NPQ(500),NQ
      COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GP(500)
      COMMON/RPERM/TKRO(500),TKRW(500),TKRG(500)
      COMMON/SAVE/OT(500),PN(500),PNP(500),PO(500)
      COMMON/VISC/AVMG,AVML,SRWM(10),UMU(10),WM(10)
      COMMON/FVOLF/ABD(10),PBO(10),NBO,IFBO,ABW(10),PEW(10),NBW,IFBW
      COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)
      EQUIVALENCE (AVMG,BG),(TLAG,VB),(PIPI,DPPI),(PIMI,DPMI),(PIPN,DPPN)
      &,(PIMN,DPMN),(TLAQ,TLAW)
      DATA RW/.666667/
C INDICATOR = 1 FOR INJECTION WELL
      I=NPQ(L)
      CALL LOOKUP(BO,PO(I),ABO,PBC,NBO,IFBO)
      CALL LOOKUP(BW,PO(I),ABW,PBW,NBW,IFBW)
      K=N*(I-1)
      IF(Y(K+1).EQ.0.0) GO TO 12
      AVMG=0.0
      DO 40 M=1,N
40    AVMG=AVMG+Y(M+K)*WM(M)
      BG=379.306*DG(I)/AVMG
12    M=1+(I-1)/NETA
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00004050

K=I-NETA*(M-1)
IF(NIND.EQ.1.OR.PWF.EQ.0.0) GO TO 11
QQ(L)=(7.07*TKRQ(I)*AKQ*HT(I))*(PO(I)-PWF)/(UMG(I)*BO*ALOG(SQR
&T(DX(K)*DY(M)/3.141593)/RW)-.75+S)
CALL BOUND(I,PIPI,PIPI,PIMN,PIMN,PO)
DPP1=PIPI-PWF
DPM1=PIM1-PWF
DPPN=PIPN-PWF
DPMN=PIMN-PWF
DPT=DPP1+DPM1+DPPN+DPMN
TLAO=(TLAMOX(I)*DPP1+SLAMOX*DPM1+TLAMOY(I)*DPPN+SLAMCY*DPMN)/DPT
TLAG=(TLAMGX(I)*DPP1+SLAMGX*DPM1+TLAMGY(I)*DPPN+SLAMGY*DPMN)/DPT
QG(L)=TLAG/TLAO*QG(L)
TLAW=(TLAMWX(I)*DPP1+SLAMWX*DPM1+TLAMWY(I)*DPPN+SLAMWY*DPMN)/DPT
QW(L)=TLAW/TLAG*QG(L)
GO TO 10
PWF=PO(I)-QG(L)*UMG(I)*BO*(ALOG(SQRT(DX(K)*DY(M)/3.141593)/RW)-.75
&+S)/(7.07*TKRQ(I)*AKQ*HT(I))
VB=DX(K)*DY(M)*HT(I)/886.905
WRITE(10,1001) I,PWF,QG(L),QW(L),NIND
1001 FORMAT(I4,4E18.6,I4)
IF(QG(L).EQ.0.0) GO TO 20
QG(L)=QG(L)*UMG(I)*BO/VB
IF(QG(L).EQ.0.0) GO TO 30
QG(L)=QG(L)*UMG(I)*BG/VB
IF(QW(L).EQ.0.0) RETURN
QW(L)=QW(L)*UMW(I)*BW/VB
RETURN
END

C
C
C SUBROUTINE LOOKUP(B,PI,A,P,KN,IFLAG)
C PURPOSE OF SUBROUTINE:
C TO DETERMINE THE VALUE OF THE DATA REQUIRED BY USING A TABLE
C OF LOOKUP OR CALCULATING THE VALUE OF THE POLYNOMIAL AS REQUIRED
C COMMON/INOUT/IN,IO,NFIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP
C DIMENSION A(10),P(10)
C IF(PI.EQ.0.0) RETURN
C IF(IFLAG.GT.1) GO TO 10
C POLYNOMIAL CALCULATION
B=0.0
DO 11 I=1,KN
11 B=B*PI+A(KN+1-I)
RETURN
C FIND RANGE

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10      J=1
      IF(P1.LT.P(1)) GO TO 21
      DO 20 I=2,KN
      IF(P1-P(I)) 30,50,20
20      J=I
21      WRITE(10,1001) P1
1001    FORMAT('IP VALUE OF',E14.6,' OUT OF RANGE',/,,' EXECUTION STOPS')
      STOP
30      IF(IFLAG.GT.2) GO TO 40
      C LINEAR INTERPOLATION
      B=A(J)+(P1-P(J))/(P(J+1)-P(J))*(A(J+1)-A(J))
      RETURN
40      C LA GRANGIAN INTERPOLATION
      B=(P1-P(J+1))/(P(J)-P(J+1))*(P1-P(J+2))/(P(J)-P(J+2))*A(J)+(P1-P(J)
      6)/(P(J+1)-P(J+2))*((P1-P(J+2))/(P(J+1)-P(J))*A(J+1)-(P1-P(J+1)))/(
      6(P(J+2)-P(J))*A(J+2))
      RETURN
      B=A(J+1)
50      RETURN
      END
C
C
C SUBROUTINE ACCP
C PURPOSE OF SUBROUTINE:
C TO DETERMINE THE ACCELERATION PARAMETER VALUES TO BE USED
C IN THE IADIP METHOD WHEN NONE ARE SPECIFIED
COMMON/FDIFF/DT,EPS,H(20),TF,THETA,ICT(250),NAP
COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCELLS,NETA,NROW
COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GT(500)
COMMON/TRIDAG/A(500),B(500),C(500),D(500),IFIRST,ILAST
COMMON/TKH/TKHX(500),TKHY(500)
EQUIVALENCE (TY,AM4),(AM3,R)
DATA TX,TY/2*0.0/
DO 60 I=IFIRST,ILAST
IF(HT(I).EQ.0.0) GO TO 60
TX=TX+TKHX(I)/HT(I)
TY=TY+TKHY(I)/HT(I)
CONTINUE
TX=TX/((ILAST-IFIRST-NIC+1)
TY=TY/((ILAST-IFIRST-NIC+1)
AM2=2.*TX/(TX+TY)
AM4=2.*TY/(TX+TY)
AM1=2.467401*AM2/NETA**2
AM3=2.467401*AM4/NROW**2
IF(AM3.LT.AM1) AM1=AM3

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22      PO(I)=D(I)
C      X-DIRECTION SWEEP
      DO 5 I=IFRST,ILAST
        KY=I+(I-1)/NETA
        KX=I-NETA*(KY-1)
        HKG=AKA*H(K)/(DX(KX)*DY(KY))
        F=THETA/DX(KX)
        CALL BOUND(I,PIPI,PIPI,PIPI,PIPI,PIPI,PNP)
        CALL CPGRV(HTX,HTY,SLAMX,SLAMY,TLAMX,TLAMY,I,NTYPE)
        A(I)=F*SLAMX
        C(I)=F*TLAMX
        B(I)=-A(I)-C(I)-VOL(I)*BI(I)/DT-HKG
        D(I)=-THETA/DY(KY)*(TLAMY*(FIPN-PO(I))-SLAMY*(PO(I)-PIMN))+
        &HTY)-F*HTX+DT(I)-HKG*PO(I)
        DO 7 I=1,NIC
          B(ICN(I))=0.0
          CALL TRIHOR(IFRST,ILAST)
          IF(NETA.EQ.NCELLS) GO TO 800
        DO 40 I=IFRST,ILAST
          PN(I)=D(I)
C      Y-DIRECTION SWEEP
      DO 6 I=IFRST,ILAST
        KY=I+(I-1)/NETA
        KX=I-NETA*(KY-1)
        HKG=AKA*H(K)/(DX(KX)*DY(KY))
        F=THETA/DY(KY)
        CALL BOUND(I,PIPI,PIPI,PIPI,PIPI,PIPI,PNP)
        CALL CPGRV(HTX,HTY,SLAMX,SLAMY,TLAMX,TLAMY,I,NTYPE)
        A(I)=F*SLAMX
        C(I)=F*TLAMX
        B(I)=-A(I)-C(I)-VOL(I)*BI(I)/DT-HKG
        D(I)=-THETA/DX(KX)*(TLAMX*(FIP1-PN(I))-SLAMX*(PN(I)-PIMN))+HT
        &X)-F*HTY+DT(I)-HKG*PN(I)
        DO 8 I=1,NIC
          B(ICN(I))=0.0
          CALL TRIVRT
        CONTINUE
      DO 50 I=IFRST,ILAST
        PNP(I)=D(I)
        CALL UPDATE
        IF(NAP.EQ.1) GO TO 73
      NC=0
C      CHECK FOR CONVERGENCE
      DO 60 I=IFRST,ILAST
        IF(ABS(PO(I)-D(I)).LE.ABS(EPS*D(I))) NC=NC+1

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73      IF(NC.LT.LAST-IFIRST+1) GO TO 70
1003    WRITE(ID,1003) TIME,M3
        FORMAT('1AT',F8.2,' DAYS, THE ',A4,'IP) PRESSURE DISTRIBUTION IS')
        DO 2 J=NETA,NCCELLS,NETA
1004    WRITE(ID,1004) (FNP(J+1-NETA),I=1,NETA)
        FORMAT('10F10.0)
2        CONTINUE
1005    IF(NAP.NE.1) WRITE(ID,1005) NCYCLE
        FORMAT('1CONVERGENCE OBTAINED IN ',I2,' CYCLES.')
        IF(TIME.GE.TF) RETURN
        GO TO 71
        END

C
C
C      SUBROUTINE LSDR(NTYPE)
C      PURPOSE OF SUBROUTINE:
C      TO PERFORM THE LINE SUCCESSIVE OVER-RELAXATION PROCEDURE
C      ON THE GIVEN GRID SYSTEM
        COMMON/FDIFF/DT,EP,S,H(20),TF,THETA,ICT(250),NAP
        COMMON/PROD/OD(50),QW(50),QG(50),NPD(50),NQ
        COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCCELLS,NETA,NROW
        COMMON/TRIDAG/A(500),B(500),C(500),D(500),IFIRST,ILAST
        COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GH(500)
        COMMON/SAVE/OT(500),PN(500),PNP(500),PO(500)
        COMMON/INPUT/IN,IO,NEIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP
        COMMON/CPLRY/PCWD(500),PCGC(500),BI(500)
        EQUIVALENCE (H(1),OMEGA)
        TIME=0.0
1001    WRITE(ID,1001) OMEGA
        FORMAT('1METHOD OF SOLUTION: LINE SUCCESSIVE OVER-RELAXATION
        &PROCEDURE (LSOR)',/,/, OMEGA='F7.4)
        DO 9 I=1,NCCELLS
9          PN(I)=D(I)
71         DO 8 I=IFIRST,ILAST
8           PO(I)=PNP(I)
            CALL IBM0B1
            TIME=TIME+DT
            ITER=0
30         NC=0
            ITER=ITER+1
            IF(ITER.GT.20) RETURN
        C      SWEEP OF EACH ROW
        DO 20 J=NETA,NCCELLS,NETA
        JMNETA=J-NETA

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DO 39 K=1,NETA
I=JNETA+K
CALL BOUND(I,PIPI,PIMI,PIPN,PIMN,PNP)
CALL CPGRV(HTX,HTY,SLAMX,SLAMY,TLAMX,TLAMY,I,NTYPE)
KY=1+(I-1)/NETA
F=THETA/DX(I-1-NTA*(KY-1))
A(K)=F*SLAMX
C(K)=F*TLAMX
B(K)=-A(K)-C(K)-F*(TLAMY+SLAMY)-VOL(I)*BI(I)/DT
D(K)=-THETA/DY(KY)*(TLAMY*PIPN+SLAMY*PIMN+HTY)-F*HTX+OT(I)
NFIRST=0
DO 38 I=1,NETA
IF(B(I).EQ.0.0) GO TO 38
IF(NFIRST.EQ.0) NFIRST=I
NLA=I
CONTINUE
CALL TRIHOR(NFIRST,NLA)
DO 20 K=1,NETA
I=JNETA+K
C CHECK FOR CONVERGENCE
IF(ABS(D(K)-PNP(I)).LE.ABS(EPS*PNP(I))) NC=NC+1
PNP(I)=PNP(I)+OMEGA*(D(K)-PNP(I))
CALL UPDATE
IF(NC.LT.NCELLS) GO TO 30
WRITE(10,1002) TIME
FORMAT('IAT',F7.1,' DAYS. THE (LSOR) PRESSURE DISTRIBUTION IS')
DO 2 J=NETA,NCCELLS,NETA
WRITE(10,1003) (PNP(J+I-NTA),I=1,NETA)
FORMAT('//.10F10.0')
CONTINUE
WRITE(10,1004) ITER
FORMAT('CONVERGENCE OBTAINED IN',I3,' ITERATIONS.')
IF(TIME.GE.TF) RETURN
GO TO 71
END

1002
1003
1004

C
C
C SUBROUTINE BOUND(I,PIPI,PIMI,PIPN,PIMN,P)
C TO DETERMINE THE VALUES TO BE USED FOR SURROUNDING CELLS
C BASED ON THEIR POSITION IN THE MODEL
COMMON/FDIFF/DT,EPS,H(20),TF,THETA,ICT(250),NAP
COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCCELLS,NETA,NROW
DIMENSION P(NCELLS)
M=(I-1)/4+1

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10      IF(B(I).EQ.0.0) GO TO 10
        DENOM=B(I)-A(I)*C(I-1)
        C(I)=C(I)/DENOM
        D(I)=(D(I)-A(I)*D(I-1))/DENOM
        CONTINUE
        N1=N*LAST-1
        DO 20 I=NFIRST,N1
          J=N1-I+NFIRST
          IF(B(I).EQ.0.0) GO TO 20
          D(J)=D(J)-C(J)*D(J+1)
        CONTINUE
        RETURN
        END

20      C
C
C      SUBROUTINE TRIVRT
C      PURPOSE OF SUBROUTINE:
C      TO PERFORM THE VERTICAL VERSION OF THE THOMAS ALGORITHM FOR
C      A TRIDIAGONAL SYSTEM
C      COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCCELLS,NETA,NROW
C      COMMON/TRIDAG/A(500),B(500),C(500),D(500),IFIRST,ILAST
        DO 20 I=IFIRST,ILAST
          IF(B(I).EQ.0.0) GO TO 21
          IF(I.LE.NETA) GO TO 30
          IMNETA=I-NETA
          DENOM=B(I)-A(I)*A(IMNETA)
          D(I)=(D(I)-A(I)*D(IMNETA))/DENOM
          IF(I.LE.NCCELLS-NETA) A(I)=C(I)/DENOM
          GO TO 20
        GO TO 20
        A(I)=C(I)/B(I)
        D(I)=D(I)/B(I)
        GO TO 20
        A(I)=0.0
        CONTINUE
        L=NCCELLS-NETA
        DO 70 I=1,L
          N=L-I+1
          IF(B(I).EQ.0.0) GO TO 70
          D(N)=D(N)-A(N)*D(NCELLS+1-I)
        CONTINUE
        RETURN
        END

70      C
C      SUBROUTINE ONCE

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C PURPOSE OF SUBROUTINE:
C TO READ IN ALL OF THE FLUID PROPERTY DATA REQUIRED FOR THE
C GIVEN SYSTEM AND TO PERFORM ALL OF THE ONE TIME CALCULATIONS
COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCELLS,NETA,NROW
COMMON/CRIT/PC(10),TC(10),TR(10),VC(10),ZC(10)/KVAL/CC(10),PRS(10)
COMMON/PCNV/A(10),B(10)/VISC/AVMG,AVML,SRWM(10),UMU(10),WM(10)
COMMON/VLIQ/DLQ(10),TA,TB,XK(10),XM(10),NC7,NCR
COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)
COMMON/INOUT/IN,IO,NFIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP
COMMON/TRIDAG/AI(500),BI(500),CI(500),D(500),E(500),IFRST,ILAST
DIMENSION W(10),Z(5000)
EQUIVALENCE (W(1),DLQ(1)),(C,ZETA,ZT),(TA,XN,PC1),(TB,XM1,ZI),(XK1,
&,TC1),(X(1),Z(1))
C IF C7+ FRACTION NOT PRESENT, NC7=N+1
1001 READ(IN,1001) NCR,NC7,N
      FORMAT(3I4)
      DO 82 I=1,N
        CALL INPUT(Y,0)
        DO 82 J=IFRST,ILAST
          Z(N*(J-1)+1)=Y(J)
          IF(NCR.EQ.N) GO TO 20
        READ(IN,1002)((NC(I+(J-1)*5),I=1,5),PC(J),TC(J),VC(J),WM(J),
&A(J),B(J),W(J),J=1,NCR)
        FORMAT(SA2,5F10.0,/,10X,3F10.0)
        J=1
        NL=I
      80 READ(IN,1001) NFRST,NLAST
      C FOR LAST GROUPED COMPONENT, NFRST=NCR+1; NLAST=-1
      C FOR PURE BETWEEN GROUPS, NFRST = FIRST OF NEXT GROUP; NLAST = LAST OF
      C NEXT GROUP
      IF(NFRST.EQ.NL) GO TO 85
      NF=NFRST-1
      DO 84 I=NL,NF
        NA=(J-1)*5
        NB=(I-1)*5
        DO 83 L=1,5
          NC(L+NA)=NC(L+NB)
        PC(J)=PC(I)
        TC(J)=TC(I)
        VC(J)=VC(I)
        ZC(J)=ZC(I)
        WM(J)=WM(I)
      83 DO 88 L=IFRST,ILAST
        Z(N*(L-1)+J)=Z(N*(L-1)+I)
      88 A(J)=A(I)

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      B(J)=B(I)
      W(J)=(.291-ZC(J))/ .08
      J=J+1
84  IF(NLAST.LE.0) GO TO 50
85  READ(IN,1002) (NC(I+(J-1)*5),I=1,5)
      ZT=0.0
      PC1=0.0
      TC1=0.0
      VC1=0.0
      ZC1=0.0
      WM1=0.0
      C SET UP FOR ALL Z'S ORIGINALLY SAME FOR EACH CELL
      DO 81 I=IFIRST,NLAST
      ZI=Z(N*(IFIRST-1)+I)
      ZT=ZT+ZI
      PC1=PC1+PC(I)*ZI
      TC1=TC1+TC(I)*ZI
      VC1=VC1+VC(I)*ZI
      ZC1=ZC1+ZC(I)*ZI
      WM1=WM1+WM(I)*ZI
81  PC(J)=PC1/ZT
      TC(J)=TC1/ZT
      VC(J)=VC1/ZT
      ZC(J)=ZC1/ZT
      WM(J)=WM1/ZT
      DO 89 L=IFIRST,ILAST
      Z(N*(L-1)+J)=ZT
89  A(J)=9400.*WM(J)*(-1.71)
      B(J)=2.*WM(J)*(-.115)
86  W(J)=(.291-ZC(J))/ .08
      NL=NLAST+1
      J=J+1
      GO TO 80
20  DO 10 J=1,N
      READ(IN,1003) (NC(I+(J-1)*5),I=1,5),PC(J),TC(J),VC(J),WM(J),
      &DLQ(J),A(J),B(J),XK1,XN,XM1,C
1003  FORMAT(SA2,6F10.0,/,10X,6F10.0)
      IF(J.GE.NC7) GO TO 10
      C CALCULATE ALANI-KENNEDY PURE COMPONENT VALUES
      XK(J)=XK1*EXP(XN/T)
      XM(J)=XM1*T+C
      CONTINUE
10  DO 90 J=1,N
80  XK1=T/TC(J)
90  TR(J)=XK1

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XMI=ZC(J)
SRWM(J)=SQRT(WM(J))
C  CALCULATE ZETA FACTOR (REID & SHERWOOD, P. 405)
ZETA=5.44085*TC(J)**.166667/SRWM(J)/PC(J)**.666667
C  CALCULATE STIEL-THODOS LOW PRESSURE, PURE GAS CORRELATION (R.&S., P.405)
IF(XK1.GT.1.5) GO TO 30
UMU(J)=34.E-5*XK1**.94/ZETA
GO TO 40
30  UMU(J)=17.78E-5*(4.58*XK1-1.67)**.625/ZETA
C  CALCULATE CONSTANTS FOR EQUILK
40  CC(J)=XMI*(.132+.25/XK1)
90  PRS(J)=10.*((90.*XMI-73.85)*XMI+16.25)*(XK1-1.)/XK1)-(-8.
    &68*(XK1-1.8+6.2*XMI)**2))
C  CALCULATE TEMPERATURE RELATED FUNCTIONS (CONSTANT)
TA=261.8082/T+10.75352
TB=2.232395E-4*T+6.225655
WRITE(IO,1004)
1004  &11X,.A,.11X,.B,.5X,.DL OR W.,/)
      DO 60 J=1,N
      NA=(J-1)*5
      WRITE(IO,1005) (NC(I+NA),I=1,5),PC(J),TC(J),VC(J),ZC(J),WM(J),A(J)
      &.B(J),W(J)
1005  &4,/)
      FFORMAT(5X,5A2.2(5X,F7.2),2(5X,F7.4),5X,F7.3,5X,F8.4,5X,F7.4,6X,F7.
      &4,/)
60  CONTINUE
      IF(NCOMP.EQ.0) RETURN
      WRITE(IO,1006)
1006  FFORMAT(10OVERALL COMPOSITION MATRIX*)
      DO 51 I=NETA,NCCELLS,NETA
      WRITE(IO,1007) (NC(J),J=1,5),(Z(N*(I+J-NETA)-9),J=1,NETA)
1007  FFORMAT(/,1X,5A2.10F10.6)
      DO 51 K=2,N
      NA=(K-1)*5
      WRITE(IO,1008) (NC(J+NA),J=1,5),(Z(N*(I+J-NETA-1)+K),J=1,NETA)
1008  FFORMAT(1X,5A2.10F10.6)
51  CONTINUE
      RETURN
      END
C
C  FUNCTION CUBEON(P,Q,R)
C  PURPOSE OF SUBPROGRAM:
C  TO DETERMINE THE SOLUTION TO A CUBIC EQUATION GIVEN THE
C  COEFFICIENTS

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EQUIVALENCE (SA,CUBEQN)
P=P/3.
C CALCULATE SMALL A FOR CUBIC EQUATION ROOT
SA=Q/3.-P*P
C CALCULATE SMALL B FOR CUBIC EQUATION ROOT
SB=P*3-.5*(P*Q-R)
C CALCULATE SQUARE ROOT FACTOR
F=SB*SB+SA**3
IF(F.LE.0.0) GO TO 10
F=SQRT(F)
C DETERMINE ROOT OF CUBIC EQUATION
IF(F+SB.LT.0.0) GO TO 30
IF(F-SB.LT.0.0) GO TO 50
CUBEQN=((-SB+F)**.333333)-((SB+F)**.333333)-P
RETURN
50 CUBEQN=(-(SB-F)**.333333)-((SB+F)**.333333)-P
RETURN
30 IF(F-SB.LT.0.0) GO TO 60
CUBEQN=((-SB+F)**.333333)+((-SB-F)**.333333)-P
RETURN
60 CUBEQN=(-(SB-F)**.333333)+((-SB-F)**.333333)-P
RETURN
C USE TRIG METHOD TO FIND ROOT
10 F=2.*SQRT(-SA)
CUBEQN=F*COS((ARCOS(2.*SB/(SA*F)))+6.283185)/3.)-P
RETURN
END

C
C
SUBROUTINE FLASH(P,L,M)
PURPOSE OF SUBROUTINE:
C TO PERFORM A FLASH CALCULATION ON A GIVEN FLUID SYSTEM
COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)
DIMENSION RK(10),Z(5000)
EQUIVALENCE (X(1),Z(1))
CALL EQUILK(P,RK,L)
IF(XL(M).GT.0.05.AND.XL(M).LT.0.95) GO TO 51
C CALCULATE FUNCTION FOR LIQUID PHASE = 0.0 AND 1.0
70 F0=0.0
F1=0.0
DO 10 I=1,N
XLN=Z(L+1)*(1.-RK(I))
F0=F0+XLN/RK(I)
F1=XLN/(1.+RK(I))
10 F1=F1+XLN

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      IF(FD.LT.0.0) GO TO 22
      IF(F1.GT.0.0) GO TO 32
C     INITIAL GUESS USING LAGRANGIAN INTERPOLATION
      XL(M)=FD/(FH-F1)*(-.5*F1/(FO-FH)+FH/(FO-F1))
51     IT=0
C     USE NEWTON-RAPHSON METHOD FOR CONVERGENCE
50     IF(IT.GT.50) GO TO 60
      IT=IT+1
      XN=0.0
      XD=0.0
      DO 40 I=1,N
        F1=Z(L+1)*(1.-RK(I))/(XLN*(1.-RK(I))+RK(I))
        XN=XN+F1
        XD=XD+F1*F1/Z(L+1)
40     XL(M)=XLN+XN/XD
        IF(XL(M).LT.0.0) XL(M)=0.0
        IF(XL(M).GT.1.0) XL(M)=1.0
        IF(ABS(XL(M)-XLN).LE.(.001*XLN)) GO TO 60
        XLN=XL(M)
      GO TO 50
22     XL(M)=0.0
20     DO 21 I=1,N
      K=L+1
      Y(K)=Z(K)
      X(K)=0.0
      RETURN
32     XL(M)=1.0
30     DO 31 I=1,N
      Y(L+1)=0.0
31     RETURN
60     IF(XL(M).EQ.0.0) GO TO 20
      IF(XL(M).EQ.1.0) GO TO 30
      DO 61 I=1,N
      K=L+1
      X(K)=Z(K)/(XL(M)+(1.-XL(M))*RK(I))
      Y(K)=RK(I)*X(K)
61     RETURN
      END
C
C     SUBROUTINE EQUILK(P,RK,L)
C     TO DETERMINE THE EQUILIBRIUM K-VALUES FOR A GIVEN SYSTEM
C     COMMON/CRT/PC(10),TC(10),TR(10),VC(10),ZC(10)/KVAL/CC(10),PRS(10)
C     COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)
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C      DIMENSION RK(N)
C      DETERMINE CONVERGENCE PRESSURE OF GIVEN SYSTEM
      CALL PCNV(PC,PCON,L)
      IF(PCON.LT.1.1*P) PCON=1.1*P
      POP=1.0-(P/PCON)
      EXPF=.00014*PCON+.08
      DO 10 I=1,N
        PR=P/PC(I)
C      DETERMINE EQUILIBRIUM K-VALUES
      RK(I)=((PRS(I)/PR)*EXP(CC(I))*(PR-PRS(I)))*(POP**((EXPF/TR(I))))
C      THE NEXT 10 ARE TEMPORARY TO CORRECT INACCURACIES IN THE CURRENT
C      K-VALUE ALGORITHM*****
      RK(1)=2.0
      RK(2)=1.075
      RK(3)=0.88
      RK(4)=0.64
      RK(5)=0.58
      RK(6)=0.40
      RK(7)=0.25
      RK(8)=0.16
      RK(9)=0.0
      RK(10)=0.0
      RETURN
      END
C
C      SUBROUTINE PCNV(PC,PCON,L)
C      PURPOSE OF SUBROUTINE:
C      TO DETERMINE THE CONVERGENCE PRESSURE FOR A GIVEN SYSTEM
      COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)
      COMMON/PCNV/A(10),B(10)/VISC/AVMG,AVML,SRWM(10),UMU(10),WM(10)
      COMMON/VLIQ/DLQ(10),TA,TB,XK(10),XM(10),NC7,NCR
      DIMENSION PC(N),W(10),Z(5000)
      EQUIVALENCE (Z(1),X(1))
      AV=0.0
      PCON=6000.
      IF(N.NE.NC7) PCON=PC(N)
      DO 10 I=1,N
        W(I)=Z(L+I)*WM(I)
        AV=AV+W(I)
      DO 20 I=1,N
C      CALCULATE WEIGHT FRACTION OF EACH COMPONENT
      W(I)=W(I)/AV
      E1=Z(L+1)
      IF(WM(1).LE.17.) E1=W(1)

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PCON=A(I)*(E1**B(I))*(AV-WM(I))+PC(I)*Z(L+1)+PCON*Z(L+N)
E1=1.
E3=1.
NN=N-1
I=1
DO 30 J=2,NN
  E1=E1-Z(L+I)
  AV=AV-WM(I)*W(I)
  E3=E3-W(I)
  I=J
30  CALCULATE CONVERGENCE PRESSURE
    PCON=PCON+(A(J)*((Z(L+J)/E1)**B(J))*(AV/E3-W(J))*E1)+PC(J)*Z(L+J)
    RETURN
    END
C
C
C SUBROUTINE CRYP RP(P,L,M)
C PURPOSE OF SUBROUTINE:
C TO DETERMINE THE CRITICAL PROPERTIES FOR A GIVEN SYSTEM
  COMMON/CRT/PC(10),TC(10),TR(10),VC(10),ZC(10)/CRITM/PCMG,PCML,TCM
  6G,TCML,VCML,VCML,ZCMG,ZCML/VISC/AVMG,AVML,SRWM(10),UMU(10),WM(10)
  COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)
  EQUIVALENCE (XI,YI,PCMG)
  AVMG=0.0
  TCMG=0.0
  ZCMG=0.0
  VCML=0.0
  AVML=0.0
  TCML=0.0
  ZCML=0.0
  VCML=0.0
  DO 10 I=1,N
    DD 10 I=1,N
  C CALCULATE LIQUID MIXTURE CRITICAL PROPERTIES
    XI=X(L+I)
    AVMG=AVMG+WM(I)*XI
    TCMG=TCMG+TC(I)*XI
    ZCML=ZCML+ZC(I)*XI
    VCML=VCML+VC(I)*XI
  C CALCULATE GAS MIXTURE CRITICAL PROPERTIES
    YI=Y(L+I)
    AVMG=AVMG+WM(I)*YI
    TCMG=TCMG+TC(I)*YI
    ZCMG=ZCMG+ZC(I)*YI
    VCML=VCML+VC(I)*YI
    IF(Y(L+I).EQ.0.0) GO TO 20
10

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	PCMG=ZCMG*10.73*TCMG/VCMG	00010360
	IF(X(L+N).EQ.0.0) GO TO 30	00010370
20	PCML=ZCML*10.73*TCML/VCML	00010380
30	CALL VOLLIQ(P,L,M)	00010390
	CALL VOLGAS(P,L,M)	00010400
	CALL VISCTY(P,L,M)	00010410
	RETURN	00010420
	END	00010430
C		00010440
C		00010450
	SUBROUTINE VOLLIQ(P,L,M)	00010460
C	PURPOSE OF SUBROUTINE:	00010470
C	TO DETERMINE THE LIQUID VOLUME FOR A GIVEN SYSTEM	00010480
	COMMON/CRIT/PC(10),TC(10),TR(10),VC(10),ZC(10)	00010490
	COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)	00010500
	COMMON/VISC/AVMG,AVML,SRWM(10),UMU(10),WM(10)	00010510
	COMMON/VLIQ/DLQ(10),TA,TB,XK(10),XM(10),NC7,NCR	00010520
	COMMON/DNSTY/DL(500),DW(500),DG(500)	00010530
	DIMENSION W(10)	00010540
	EQUIVALENCE (W(1),DLQ(1)),(BM,XC7),(XI,A1,S),(Q,B),(R,A3,C),(WMC7,	00010550
	DC1),(DC7,C,C2),(A,A4)	00010560
	DL(M)=0.0	00010570
	IF(X(L+1).EQ.0.0) RETURN	00010580
	IF(NCR.NE.N) GO TO 40	00010590
	AM=0.0	00010600
	BM=0.0	00010610
	IF(NC7.GT.N) GO TO 20	00010620
	DC7=0.0	00010630
	WMC7=0.0	00010640
	DO 30 I=NC7,N	00010650
	XI=X(L+I)	00010660
	XC7=XC7+XI	00010670
	DC7=DC7+DLQ(I)*XI	00010680
30	WMC7=WMC7+WM(I)*XI	00010690
C	DETERMINE C7+ FRACTION MOLECULAR WEIGHT AND DENSITY	00010700
	WMC7=WMC7/XC7	00010710
	DC7=DC7/XC7	00010720
C	CALCULATE ALANI-KENNEDY C7+ FRACTION A AND B VALUES	00010730
	AM=XC7*EXP(((7.310446E-6*WMC7-5.967829E-2/DC7+3.840599E-3)*WMC7+TA)	00010740
	BM=XC7*((3.499274E-2-1.018528/DC7)*WMC7-1.165471E-1*DC7+TB)	00010750
20	NN=NC7-1	00010760
	DO 10 I=1,NN	00010770
	XI=X(L+I)	00010780
	AM=AM+XK(I)*XI	00010790
10	BM=BM+XM(I)*XI	00010800

	A1=-BM-10.73*T/P	00010810
	AM=AM/P	00010820
	BM=-BM*AM	00010830
	DL(M)=AVML/CUBEQN(A1,AM,BM)	00010840
	RETURN	00010850
40	C1=0.0	00010860
	C2=0.0	00010870
	B=0.0	00010880
	A1=0.0	00010890
	A2=0.0	00010900
	A3=0.0	00010910
	A4=0.0	00010920
	DO 50 I=1,N	00010930
	J=L+I	00010940
	AM=115.133*TC(I)/PC(I)	00010950
	A1=A1+X(J)*(AM*TC(I)*(.25913-.031314*W(I)))*.5	00010960
	A2=A2+X(J)*(AM*(.0249+.15369*W(I)))*.5	00010970
	TC2=TC(I)**2	00010980
	BM=AM*TC2	00010990
	A3=A3+X(J)*(BM*(.2015+.21642*W(I)))*.5	00011000
	A4=A4+X(J)*TC2*(BM*.042*W(I))*.5	00011010
	B=B+X(J)*AM*.009152	00011020
	BM=BM*.64277/PC(I)	00011030
	C1=C1+X(J)*(BM*TC(I)**.5*(1.-W(I)))*.333333	00011040
50	C2=C2+X(J)*(BM*TC2*(.302584+1.53486*W(I)))*.333333	00011050
	A=A1*A1-A2*A2*T+(A4*A4/T**4+A3*A3)/T	00011060
	C=C1**3/T**.5+C2**3/T**2	00011070
	R=(A*B-C)/P	00011080
	S=-10.73*T/P	00011090
	Q=A/P+(S-B)*B	00011100
	DL(M)=AVML/CUBEQN(S,Q,R)	00011110
	RETURN	00011120
	END	00011130
C		00011140
C		00011150
	SUBROUTINE VOLGAS(P,L,M)	00011160
C	PURPOSE OF SUBROUTINE:	00011170
C	TO DETERMINE THE VAPOR VOLUME FOR A GIVEN SYSTEM	00011180
	COMMON/CRITM/PCMG,PCML,TCMG,TCML,VCMG,VCML,ZCMG,ZCML	00011190
	COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)	00011200
	COMMON/DNSTY/DL(500),DW(500),DG(500)	00011210
	COMMON/INOUT/IN,IO,NFIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP	00011220
	COMMON/TRIDAG/A1(500),B1(500),C(500),D(500),IFRST,ILAST	00011230
	COMMON/FVOLF/ABO(10),PBO(10),NBO,IFBO,ABW(10),PBW(10),NBW,IFBW	00011240
	COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GH(500)	00011250

	COMMON/SATN/SW(500),SG(500),SQ(500),CF	00011260
	COMMON/PROD/QO(50),QW(50),QG(50),NPQ(50),NQ	00011270
	COMMON/VISC/AVMG,AVML,SRWM(10),UMU(10),WM(10)	00011280
	DIMENSION A(36),B(12)	00011290
	EQUIVALENCE (XX,YY,BM),(X2,Y2,ZZ),(BO,BG,BW)	00011300
	DATA A/2.14335,.331235,.105729,-.052184,.019704,-5.30959E-3,.0831700011310	
	&62,-.134036,-.0503937,.0443121,-.0263833,8.91783E-3,-.021467,.066800011320	
	&81,5.09248E-3,-.0193295,.0192621,-.0108948,-8.71403E-4,-.0271743,.00011330	
	&015513,5.89725E-3,-.0115354,9.55939E-3,4.28463E-3,8.85123E-3,-7.3100011340	
	&819E-3,1.53667E-3,4.29101E-3,-6.0114E-3,-1.65953E-3,-2.15209E-3,2.00011350	
	&696E-3,-2.83268E-3,-8.13025E-4,3.11752E-3/	00011360
	DATA B(1),B(7),GIF,OIP,WIP/2*7.071068E-1,3*0.0/	00011370
	DG(M)=0.0	00011380
	IF(HT(M).EQ.0.0) RETURN	00011390
	CALL LOOKUP(BW,P,ABW,PBW,NBW,IFBW)	00011400
	DW(M)=63.698/BW	00011410
	IF(M.NE.IFRST) GO TO 11	00011420
	GIP=0.0	00011430
	OIP=0.0	00011440
	WIP=0.0	00011450
	VTOT=0.0	00011460
11	IF(Y(L+1).EQ.0.0) GO TO 20	00011470
	XX=1.351351E-1*P/PCMG-1.013514	00011480
	X2=XX*XX	00011490
	B(2)=1.224745*XX	00011500
	B(3)=2.371709*X2-7.905695E-1	00011510
	B(4)=(4.677073*X2-2.806244)*XX	00011520
	B(5)=(9.280775*X2-7.95495)*X2+.795495	00011530
	B(6)=((1.846851E1*X2-2.052057E1)*X2+4.397265)*XX	00011540
	YY=1.052632*T/TCMG-2.105263	00011550
	Y2=YY*YY	00011560
	B(8)=1.224745*YY	00011570
	B(9)=2.371709*Y2-7.905695E-1	00011580
	B(10)=(4.677073*Y2-2.806244)*YY	00011590
	B(11)=(9.280775*Y2-7.95495)*Y2+.795495	00011600
	B(12)=((1.846851E1*Y2-2.052057E1)*Y2+4.397265)*YY	00011610
	ZZ=0.0	00011620
	DO 10 K=1,6	00011630
	BM=B(K)	00011640
	J=6*K-6	00011650
	DO 10 LL=1,6	00011660
10	ZZ=ZZ+A(J+LL)*BM*B(LL+6)	00011670
	DG(M)=AVMG*P/(ZZ*10.73*T)	00011680
20	IF(NFIP.EQ.0) RETURN	00011690
C	CALCULATE AND PRINT FLUIDS IN PLACE	00011700


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21      VTOT=VTOT+VOL(M)
      WIP=WIP+VOL(M)*SW(M)/(5.6146*BW)
      IF(X(L+1).EQ.0.0) GO TO 21
      CALL LOOKUP(BO.P,ABO,PBO,NBC,IFBO)
      OIP=OIP+VOL(M)*SO(M)/(5.6146*BO)
      IF(Y(L+1).EQ.0.0) GO TO 22
      BG=379.306*DG(M)/AVMG
      GIP=GIP+VOL(M)*SG(M)/BG
      IF(M.NE.ILAST) RETURN
      WRITE(10,1001) VTOT,GIP,OIP,WIP
      FORMAT(11TOTAL RESERVOIR PORE VOLUME =,E14.6,, CUBIC FEET,,//,, G00011810
1001  GAS IN PLACE =,E14.6,, STANDARD CUBIC FEET,,//,, OIP IN PLACE =,E00011820
      ,E14.6,, STOCK TANK BARRELS,,//,, WATER IN PLACE =,E14.6,, STOCK TA000011830
      ENK BARRELS,,//,3E18.6)
      RETURN
      END

C
C
C      SUBROUTINE VISCY(P,L,M)
C      PURPOSE OF SUBROUTINE:
C      TO DETERMINE THE LIQUID AND VAPOR VISCOSITIES FOR A GIVEN SYSTEM
      COMMON/CRITM/PCMG,PCML,TCMG,TCML,VCMG,VCML,ZCMG,ZCML
      COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)
      COMMON/VISC/AVMG,AVML,SRWM(10),UMU(10),WM(10)
      COMMON/VSCY/UMD(500),UMG(500),DGM(500)
      COMMON/DNSTY/DL(500),DW(500),DG(500)
      COMMON/WTRV/AUM(10),PUW(10),NUW,IFUW
      COMMON/EQVLENCE (DRMG,XD),(DRML,XDP),(XN,UMM)
      CALL LOOKUP(UMW(M),P,AUM,PUW,NUW,IFUW)
      IF(Y(L+1).NE.0.0) GO TO 40
      UMM=0.0
      GO TO 30
      XDP=0.0
      XN=0.0
      DO 10 I=1,N
      XD=SRWM(I)*Y(L+1)
      XN=XN+XD*UMU(I)
      XDP=XDP+XD
10  C      CALCULATE HERNING-ZIPPERER LOW PRESSURE GAS MIXTURE VISCOSITY (REID
C
C      SHERWOOD, P. 423)
      UMM=XN/XDP
C      CALCULATE REDUCED DENSITIES
      UMO(M)=0.0
      IF(X(L+N).EQ.0.0) GO TO 20
      DRML=VCML/(AVML/DL(M))
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C  CALCULATE LIQUID VISCOSITY AT RESERVOIR CONDITIONS USING JOSSI-STIEL-00012160
C  THODOS CORRELATION (REID & SHERWOOD, P. 413) 00012170
    UMO(M)=((((0.0093324*DRML-.040758)*DRML+.058533)*DRML+.023364)*DRM00012180
    &L+.1023)**4-.0001)/5.44085/TCML**1.66667*SQRT(AVML)*PCML**00012190
    &UMM 00012200
    UMG(M)=0.0 00012210
    IF(Y(L+1).EQ.0.0) RETURN 00012220
20  DRMG=VCMG/(AVMG/DG(M)) 00012230
C  CALCULATE GAS VISCOSITY AT RESERVOIR CONDITIONS USING DEAN-STIEL 00012240
C  CORRELATION (REID & SHERWOOD, P. 426) 00012250
    UMG(M)=UMM+1.98498E-5*(EXP(1.439*DRMG)-EXP(-1.111*DRMG**1.858))/TC00012260
    &MG**1.66667*SQRT(AVMG)*PCMG**00012270
    RETURN 00012280
    END 00012290
C 00012300
C 00012310
    SUBROUTINE SATRN 00012320
C  PURPOSE OF SUBROUTINE: 00012330
C  TO DETERMINE THE OIL, GAS, AND WATER SATURATIONS FOR A GIVEN SYSTEM 00012340
    COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCELLS,NETA,NROW 00012350
    COMMON/SATN/SW(500),SG(500),SO(500),CF 00012360
    COMMON/TRIDAG/A(500),B(500),C(500),D(500),IFRST,ILAST 00012370
    COMMON/SAVE/OT(500),PN(500),PNP(500),PO(500) 00012380
    COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GH(500) 00012390
    COMMON/FD/IFF/DT,EPS,H(20),TF,THETA,ICT(250),NAP 00012400
    COMMON/IBMBTX/TLAMOX(500),TLAMGX(500),TLAMWX(500) 00012410
    COMMON/IBMBTY/TLAMOY(500),TLAMGY(500),TLAMWY(500) 00012420
    COMMON/PROD/QO(50),QW(50),QG(50),NPQ(50),NQ 00012430
    COMMON/DNSTY/DL(500),DW(500),DG(500) 00012440
    COMMON/INOUT/IN,IO,NFIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NFLKUP 00012450
    DATA N1,N2,N3/'OIL ','GAS ','H2O '/ 00012460
    J=1 00012470
    KQ=1 00012480
    DO 10 I=IFRST,ILAST 00012490
    IF(ICN(J).NE.I) GO TO 20 00012500
    J=J+1 00012510
    GO TO 10 00012520
20  PHIOLD=PHI(I) 00012530
    PHI(I)=PHIOLD*(1.+CF*(PNP(I)-PO(I))) 00012540
    VOL(I)=PHIOLD*VOL(I)/PHI(I) 00012550
    CALL BOUND(I,PIP1,PIM1,PIP1N,PIMN,PNP) 00012560
    KY=1+(I-1)/NETA 00012570
    BQO=0.0 00012580
    BQW=0.0 00012590
    PFAC=(PHI(I)-PHIOLD)*DT/PHIOLD 00012600

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      IF(NP0(KQ).NE.1) GO TO 12
      IF(DL(I).NE.0.0) BQ0=Q0(KQ)*DT/(VOL(I)*DL(I))
      IF(DW(I).NE.0.0) BQW=QW(KQ)*DT/(VOL(I)*DW(I))
      KQ=KQ+1
12    C2=DT/VOL(I)/DY(KY)
      C1=DT/VOL(I)/DX(I-NEA*(KY-1))
      IF(I.LE.NEA) GO TO 41
      SLAMOY=TLAMOY(I-NEA)
      SLAMWY=TLAMWY(I-NEA)
      SLAMOX=TLAMOX(I-1)
      SLAMWX=TLAMWX(I-1)
      GO TO 45
41    SLAMOY=0.0
      SLAMWY=0.0
      IF(I.NE.IFRST) GO TO 42
      SLAMOX=0.0
      SLAMWX=0.0
45    SO(I)=C1*(TLAMOX(I)*(PIPI-PNP(I))-SLAMOX*(PNP(I)-PIMI))+C2*(TLAMOY
      &(I)*(PIPN-PNP(I))-SLAMOY*(PNP(I)-PIMN))-BQ0-SO(I)*PFAC+SD(I)
      SW(I)=C1*(TLAMWX(I)*(PIPI-PNP(I))-SLAMWX*(PNP(I)-PIMI))+C2*(TLAMWY
      &(I)*(PIPN-PNP(I))-SLAMWY*(PNP(I)-PIMN))-BQW-SW(I)*PFAC+SW(I)
      IF(SO(I).LT.1.E-5) SO(I)=0.0
      IF(SW(I).LT.1.E-5) SW(I)=0.0
      SG(I)=1.0-SW(I)-SO(I)
      IF(SG(I).LT.1.E-5) SG(I)=0.
      CONTINUE
10    IF(NSAT.EQ.0) RETURN
      WRITE(IO,1001)
1001  FORMAT('1SATURATION MATRICES')
      DO 51 I=NEA,NCELLS,NEA
      WRITE(IO,1002) N1.(SO(I+J-NEA),J=1,NEA)
1002  FORMAT('/',1X,A4,10F10.5)
      WRITE(IO,1003) N2.(SG(I+J-NEA),J=1,NEA)
1003  FORMAT(1X,A4,10F10.5)
      WRITE(IO,1003) N3.(SW(I+J-NEA),J=1,NEA)
51    CONTINUE
      RETURN
      END

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C
C
C  SUBROUTINE 18MOB1
C  TO DETERMINE THE INTERBLOCK MOBILITIES FOR A GIVEN SYSTEM
C  COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCELLS,NEA,NROW
C  COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GH(500)

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	COMMON/SATN/SW(500),SG(500),SD(500),CF	00013060
	COMMON/FLUID3/AKROG(10),AKROW(10),AKRG(10),AKRW(10)	00013070
	COMMON/FLUID4/SKROG(10),SKROW(10),SKRG(10),SKRW(10)	00013080
	COMMON/IBMBTX/TLAMOX(500),TLAMGX(500),TLAMWX(500)	00013090
	COMMON/IBMBTY/TLAMOY(500),TLAMGY(500),TLAMWY(500)	00013100
	COMMON/TKH/TKHX(500),TKHY(500)	00013110
	COMMON/PERMF/NKROG,IFKROG,NKROW,IFKROW,NKRG,IFKRG,NKRW,IFKRW	00013120
	COMMON/RPERM/TKRO(500),TKRW(500),TKRG(500)	00013130
	COMMON/TRIDAG/A(500),B(500),C(500),D(500),IFRST,ILAST	00013140
	COMMON/VSCTY/UMO(500),UMG(500),UMW(500)	00013150
	COMMON/SAVE/OT(500),PN(500),PNP(500),PO(500)	00013160
	COMMON/INOUT/IN,IO,NFIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP	00013170
	DATA NX,NY,N1,N2,N3/'X-DI','Y-DI','OIL ','GAS ','H2O '/	00013180
	J=1	00013190
C	CALCULATE KRO FOR EACH CELL USING STONE EQUATION	00013200
	DO 10 I=IFRST,ILAST	00013210
	IF(ICN(J).NE.I) GO TO 15	00013220
	J=J+1	00013230
	GO TO 10	00013240
15	CALL LOOKUP(TKROW,SW(I),AKROW,SKROW,NKROW,IFKROW)	00013250
	CALL LOOKUP(TKRW(I),SW(I),AKRW,SKRW,NKRW,IFKRW)	00013260
	CALL LOOKUP(TKROG,SG(I),AKRG,SKRG,NKRG,IFKRG)	00013270
	CALL LOOKUP(TKRG(I),SG(I),AKRG,SKRG,NKRG,IFKRG)	00013280
	TKRO(I)=(TKROW+TKRW(I))*(TKROG+TKRG(I))-(TKRW(I)+TKRG(I))	00013290
	IF(TKRO(I).LT.0.0) TKRO(I)=0.0	00013300
10	CONTINUE	00013310
C	CALCULATE INTERBLOCK MOBILITIES FOR EACH CELL	00013320
	J=1	00013330
	LL=NCELLS-NETA+1	00013340
	DO 30 I=IFRST,ILAST	00013350
	IF(ICN(J).NE.I) GO TO 20	00013360
	J=J+1	00013370
	GO TO 30	00013380
20	KY=1+(I-1)/NETA	00013390
	L=KY*NETA	00013400
	KX=I-NETA*(KY-1)	00013410
	M=L-NETA+1	00013420
	IF(L.GT.ILAST) L=ILAST	00013430
	IF(M.LT.IFRST) M=IFRST	00013440
	CALL IBMOB2(DX,TOX,TGX,TWX,I,KX,L,M,1)	00013450
	CALL IBMOB2(DY,TOY,TGY,TWY,I,KX,LL,KY,NETA)	00013460
	IF(UMO(I).EQ.0.0) GO TO 11	00013470
	TLAMOX(I)=TOX/UMG(I)	00013480
	TLAMOY(I)=TOY/UMO(I)	00013490
	GO TO 12	00013500

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11      TLAMOX(I)=0.0
12      IF(UMG(I).EQ.0.0) GO TO 13
13      TLAMGX(I)=TGX/UMG(I)
14      TLAMGY(I)=TGY/UMG(I)
15      GO TO 14
16      TLAMGX(I)=0.0
17      TLAMGY(I)=0.0
18      TLAMWX(I)=TWX/UMW(I)
19      TLAMWY(I)=TWY/UMW(I)
20      IF(I.EQ.L) GO TO 41
21      IF(HT(I+1).EQ.0.0) GO TO 41
22      IF(I.EQ.1) GO TO 50
23      IF(PNP(I-1).GT.PNP(I)) GO TO 61
24      IF(HT(I+NETA).EQ.0.0) GO TO 51
25      IF(I.LE.NETA) GO TO 31
26      IF(PNP(I-NETA).GT.PNP(I)) GO TO 71
27      GO TO 31
28      TLAMOX(I)=0.0
29      TLAMGX(I)=0.0
30      TLAMWX(I)=0.0
31      GO TO 50
32      TLAMOX(I)=0.0
33      TLAMGX(I)=0.0
34      TLAMWY(I)=0.0
35      GO TO 31
36      TLAMOX(I)=TLAMOX(I-1)
37      TLAMGX(I)=TLAMGX(I-1)
38      TLAMWX(I)=TLAMWX(I-1)
39      GO TO 50
40      TLAMOX(I)=TLAMOX(I-NETA)
41      TLAMGY(I)=TLAMGY(I-NETA)
42      TLAMWY(I)=TLAMWY(I-NETA)
43      TLAMGX(I)=TLAMGX(I)*TKHX(I)
44      TLAMWX(I)=TLAMWX(I)*TKHX(I)
45      TLAMGY(I)=TLAMGY(I)*TKHY(I)
46      TLAMWY(I)=TLAMWY(I)*TKHY(I)
47      CONTINUE
48      IF(NLMDA.EQ.0) RETURN
49      WRITE(ID,1001) NX
50      FORMAT('1CROSS SECTIONAL AREA * 'A4,'RECTION MOBILITIES')
51      DO 53 L=NETA,NCCELLS,NETA
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	IF(TW.LT.0.0) TW=0.0	00014410
	IF(TG.LT.0.0) TG=0.0	00014420
	RETURN	00014430
70	IF(PNP(I).GT.PNP(I+N)) GO TO 80	00014440
	DO 71 J=1,NQ	00014450
	IF(I.EQ.NPQ(J).OR.I+N.EQ.NPQ(J)) GO TO 20	00014460
71	CONTINUE	00014470
	IF(HT(I+N).EQ.0.0) GO TO 20	00014480
	F=D(KX)/(D(KX)+D(KX+1))	00014490
	TO=TKRO(I)-F*(TKRO(I+N)-TKRO(I))	00014500
	TW=TKRW(I)-F*(TKRW(I+N)-TKRW(I))	00014510
	TG=TKRG(I)-F*(TKRG(I+N)-TKRG(I))	00014520
	GO TO 61	00014530
80	IF(I.EQ.M) GO TO 20	00014540
	IF(PNP(I).GE.PNP(I-N)) GO TO 20	00014550
	DO 81 J=1,NQ	00014560
	IF(I-N.EQ.NPQ(J)) GO TO 20	00014570
81	CONTINUE	00014580
	GO TO 50	00014590
40	TO=TKRO(I-N)	00014600
	TW=TKRW(I-N)	00014610
	TG=TKRG(I-N)	00014620
	RETURN	00014630
	END	00014640
C		00014650
C		00014660
	SUBROUTINE OLDT(NTYPE)	00014670
C	PURPOSE OF SUBROUTINE:	00014680
C	TO CALCULATE THE VALUE OF AN INTERMEDIATE FINITE DIFFERENCE	00014690
C	TERM AT THE OLD TIME VALUES	00014700
	COMMON/FDIFF/DT, EPS, H(20), TF, THETA, ICT(250), NAP	00014710
	COMMON/SYSTEM/DX(20), DY(20), ICN(30), METHOD, NIC, NCELLS, NETA, NROW	00014720
	COMMON/PROD/QO(50), QW(50), QG(50), NPQ(50), NQ	00014730
	COMMON/IBMBTX/TLAMOX(500), TLAMGX(500), TLAMWX(500)	00014740
	COMMON/IBMBTY/TLAMOY(500), TLAMGY(500), TLAMWY(500)	00014750
	COMMON/ROCK/PHI(500), HT(500), ZEL(500), VOL(500), GH(500)	00014760
	COMMON/DNSTY/DL(500), DW(500), DG(500)	00014770
	COMMON/CPLRY/PCWO(500), PCGC(500), B1(500)	00014780
	COMMON/TRIDAG/A(500), B(500), C(500), D(500), IFRST, ILAST	00014790
	COMMON/SAVE/OT(500), PN(500), PNP(500), PO(500)	00014800
	COMMON/INOUT/IN, IO, NFIP, NLMDA, NSAT, NPOT, NCOMP, NTKH, NPLKUP	00014810
	EQUIVALENCE (GHDL, GHDW, GHDG)	00014820
	DATA CTX, CTY, GTX, GTY/4*0.0/	00014830
	WRITE(IO,1004)	00014840
1004	FORMAT('1CELL # PWF',5X,'QO',7X,'QG',7X,'QW',7X,'INJ.OR PROD')	00014850

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C   TEMPORARY: FOR SAMPLE PROBLEM WITH MANY TIME STEPS ONLY*****
      IF(DT.LE.0.0) GO TO 12
      PWF=1500.0
      AKQ=1.0
      S=0.0
      I=1
      NIND=0
      CALL SDRSNK(AKQ,PWF,S,I,NIND)
      GO TO 13
C   END OF TEMPORARY*****
12  READ(IN,1001) NQ,DT
1001 FORMAT(I4,F10.0)
      DO 11 I=1,NQ
1002  READ(IN,1002) NIND,NPQ(I),GD(I),QG(I),QW(I),PWF,S,AKQ
      FORMAT(2I4,6F10.0)
      CALL SDRSNK(AKQ,PWF,S,I,NIND)
11   CONTINUE
13   KG=1
      J=1
      DO 10 I=IFIRST,ILAST
      IF(ICN(J).NE.I) GO TO 30
      J=J+1
      OT(I)=0.0
      GO TO 10
30   CALL BOUND(I,PIPI,PIMI,PIPN,PIMN,PO)
      TLX=(TLAMDX(I)+TLAMWX(I))+TLAMGX(I))*((PIPI-PO(I))
      TLY=(TLAMOY(I)+TLAMWY(I))+TLAMGY(I))*((PIPN-PO(I))
      IF(I.LE.NETA) GO TO 41
      SLAMDY=TLAMOY(I-NETA)
      SLAMGY=TLAMGY(I-NETA)
      SLAMWX=TLAMWX(I-NETA)
      SLAMGX=TLAMGX(I-1)
      SLAMWX=TLAMWX(I-1)
      GO TO 45
42   SLAMDY=0.0
      SLAMGY=0.0
      SLAMWX=0.0
      SLAMGX=0.0
      IF(I.NE.IFIRST) GO TO 42
41   SLAMDY=0.0
      SLAMGY=0.0
      SLAMWX=0.0
      SLAMGX=0.0
      SLX=(SLAMDY+SLAMGX+SLAMWX)*((PO(I)-PIMI)
      SLY=(SLAMGY+SLAMGX+SLAMWY)*((PO(I)-PIMN)
      IF(NTYPE) 31,20,50

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40      OT(I)=F/DY(KY)*{(TLY-SLY+GTY+CTY)+F/DX(I-NETA*{(KY-1))*{(TLX-SLX+GTX+00015760
&CTX)-VOL(I)*B1(I)*PO(I)/DT+B2                                00015770
10      CONTINUE                                                00015780
      RETURN                                                    00015790
      END                                                        00015800
C                                                            00015810
C                                                            00015820
      SUBROUTINE CPGRV(HTX,HTY,SLAMX,SLAMY,TLAMX,TLAMY,I,NTYPE) 00015830
C  PURPOSE OF SUBROUTINE:                                       00015840
C  TO DETERMINE THE VALUES OF THE CAPILLARY AND GRAVITY TERMS OF 00015850
C  THE FINITE DIFFERENCE EQUATION                               00015860
      COMMON/IBMTX/TLAMOX(500),TLAMGX(500),TLAMWX(500)          00015870
      COMMON/IBMTY/TLAMOY(500),TLAMGY(500),TLAMWY(500)          00015880
      COMMON/DNSTY/DL(500),DW(500),DG(500)                      00015890
      COMMON/CPLRY/PCWO(500),PCGO(500),B1(500)                 00015900
      COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCELLS,NETA,NROW 00015910
      COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GH(500)   00015920
      EQUIVALENCE (PCWIP1,PCGIP1,DLIP1,DWIP1,DGIP1),(PCWIM1,PCGIM1,DLIM1,00015930
&,DWIM1,DGIM1),(PCWIPN,PCGIPN,DLIPN,DWIPN,DGIPN),(PCWIMN,PCGIMN,DLIMN,00015940
&PN,DWIPN,DGIPN),(PCWIMN,PCGIMN,DLIMN,DWIMN,DGIMN),(H7,H3),(H17,H1300015950
&),(H9,H1),(H19,H11),(H10,H4),(H20,H14),(GHD1,GHDW,GHDG)      00015960
      DATA H2,H8,H12,H18/4*0.0/                                00015970
      IF(HT(I).EQ.0.0) GO TO 10                                  00015980
      IF(I.LE.NETA) GO TO 41                                     00015990
      SLAMOY=TLAMOY(I-NETA)                                     00016000
      SLAMGY=TLAMGY(I-NETA)                                     00016010
      SLAMWY=TLAMWY(I-NETA)                                     00016020
42      SLAMOX=TLAMOX(I-1)                                       00016030
      SLAMGX=TLAMGX(I-1)                                       00016040
      SLAMWX=TLAMWX(I-1)                                       00016050
      GO TO 45                                                    00016060
41      SLAMOY=0.0                                                00016070
      SLAMGY=0.0                                                00016080
      SLAMWY=0.0                                                00016090
      IF(I.NE.IFRST) GO TO 42                                    00016100
      SLAMOX=0.0                                                00016110
      SLAMGX=0.0                                                00016120
      SLAMWX=0.0                                                00016130
45      IF(NTYPE) 70,50,90                                       00016140
C  CONSIDER CAPILLARY EFFECTS                                   00016150
90      CALL EBOUND(PCWIP1,PCWIM1,PCWIPN,PCWIMN,PCWO)           00016160
      H7=TLAMWY(I)*(PCWIPN-PCWO(I))                             00016170
      H8=SLAMWY*(PCWO(I)-PCWIMN)                               00016180
      H17=TLAMWX(I)*(PCWIP1-PCWO(I))                           00016190
      H18=SLAMWX*(PCWO(I)-PCWIM1)                              00016200

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CALL EBOUND(PCGIP1,PCGIM1,PCGIPN,PCGIMN,PCGO)
H9=TLAMGY(I)*(PCGIPN-PCGO(I))
H10=SLAMGY*(PCMO(I)-PCGIMN)
H19=TLAMGX(I)*(PCGIP1-PCGO(I))
H20=SLAMGX*(PCGO(I)-PCGIM1)
H8=H8-H7+H9-H10
H18=H18-H17+H19-H20
IF(NTYPE,NE.2) GO TO 50
C CONSIDER GRAVITY EFFECTS
70 CALL EBOUND(GHIP1,GHIM1,GHIPN,GHIMN,GH)
CALL EBOUND(DLIP1,DLIM1,DLIPN,DLIMN,DL)
GHD=GH(I)*DL(I)
H1=TLAMOY(I)*(GHIPN*DLIPN-GHD)
H2=SLAMOY*(GHDL-GHIMN*DLIMN)
H11=TLAMOX(I)*(GHIP1*DLIP1-GHD)
H12=SLAMOX*(GHDL-GHIM1*DLIM1)
CALL EBOUND(DWIP1,DWIM1,DWIPN,DWIMN,DW)
GHDW=GH(I)*DW(I)
H3=TLAMWY(I)*(GHIPN*DWIPN-GHDW)
H4=SLAMWY*(GHDW-GHIMN*DWIMN)
H13=TLAMWX(I)*(GHIP1*DWIP1-GHDW)
H14=SLAMWX*(GHDW-GHIM1*DWIM1)
CALL EBOUND(DGIP1,DGIM1,DGIPN,DGIMN,DG)
GHDG=GH(I)*DG(I)
H5=TLAMGY(I)*(GHIPN*DGIPN-GHDG)
H6=SLAMGY*(GHDG-GHIMN*DGIMN)
H15=TLAMGX(I)*(GHIP1*DGIP1-GHDG)
H16=SLAMGX*(GHDG-GHIM1*DGIM1)
H2=H2-H3-H1+H4-H5+H6
H12=H12-H13-H11+H14-H15+H16
H1X=H12+H18
H1Y=H2+H8
TLAMX=TLAMOX(I)+TLAMGX(I)+TLAMWX(I)
SLAMX=SLAMOX+SLAMGX+SLAMWX
TLAMY=TLAMOY(I)+TLAMGY(I)+TLAMWY(I)
SLAMY=SLAMOY+SLAMGY+SLAMWY
RETURN
10 HTX=0.0
HTY=0.0
SLAMX=0.0
SLAMY=0.0
TLAMX=0.0
TLAMY=0.0
RETURN
END

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00016210
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C
C
C SUBROUTINE UPDATE
C PURPOSE OF SUBROUTINE:
C TO UPDATE ALL VALUES AT THE NEW PRESSURE
COMMON/SATN/SW(500),SG(500),SO(500),CF
COMMON/CPLRV/PCWO(500),PCGO(500),BI(500)
COMMON/PCAP0/APCO(10),PPCO(10),NPCO,IFPCO
COMMON/PCAPG/APCG(10),PPCG(10),NPCG,IFPCG
COMMON/ROCK/PHI(500),HT(500),ZEL(500),VOL(500),GH(500)
COMMON/DNSTV/DL(500),DW(500),DG(500)
COMMON/COMP/T,XL(500),X(5000),Y(5000),N,NC(50)
COMMON/TRIDAG/A(500),B(500),C(500),D(500),IFRST,ILAST
COMMON/WTRV/AUM(10),PUW(10),NUW,IFUW
COMMON/INOUT/IN,IO,NEIP,NLMDA,NSAT,NPOT,NCOMP,NTKH,NPLKUP
COMMON/SYSTEM/DX(20),DY(20),ICN(30),METHOD,NIC,NCELLS,NETA,NROW
COMMON/SAVE/OT(500),PN(500),PNP(500),PO(500)
COMMON/COMPI/ACO(10),ACW(10),ACG(10),PCD(10),PCW(10),PCG(10)
COMMON/COMPI/NCO,NCW,NCG,IFCO,IFCW,IFCG
COMMON/COMPI/POTL(500),POTW(500),POTG(500),Z(5000)
DATA N1,N2,N3,'OIL','GAS','H2O'/'
EQUIVALENCE (X(1),Z(1)),(POTL(1),A(1)),(POTW(1),B(1)),(POTG(1),C(1))
6))
DO 10 I=IFRST,ILAST
POTL(I)=PNP(I)-DL(I)*GH(I)
POTG(I)=PNP(I)+PCGO(I)-DG(I)*GH(I)
POTW(I)=PNP(I)+PCWO(I)-DW(I)*GH(I)
IF(NPOT.EQ.0) GO TO 41
WRITE(10,1001)
FORMAT(1,POTENTIAL MATRICES.)
DO 42 I=NETA,NCELLS,NETA
WRITE(10,1002) N1,(POTL(I+J-NETA),J=1,NETA)
FORMAT(//,1X,A4,10F10.3)
WRITE(10,1003) N2,(POTG(I+J-NETA),J=1,NETA)
FORMAT(1X,A4,10F10.3)
WRITE(10,1003) N3,(POTW(I+J-NETA),J=1,NETA)
CONTINUE
J=1
DO 11 I=IFRST,ILAST
IF(ICN(J).NE.I) GO TO 12
J=J+1
GO TO 11
CALL BOUND(I,POTLP1,POTLM1,POTLPN,POTLMN,POTL)
CALL CPGRV(HTX,HTY,SLAMX,SLAMY,TLAMX,TLAMY,I,0)
C1=DL(I)*(TLAMX*(POTLP1-POTL(I))-SLAMX*(POTL(I)-POTLM1)+TLAMY*(POT
00016660
00016670
00016680
00016690
00016700
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00017100
00017110

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&LPN-POTL(I))-SLAMY*(POTL(I)-POTLMN))
CALL EBOUND(POTGP1,POTGM1,POTGPN,POTGMN,POTG)
C2=DG(I)*(TLAMX*(POTGP1-POTG(I))-SLAMX*(POTG(I)-POTGMN))+TLAMY*(POT
&GPN-POTG(I))-SLAMY*(POTG(I)-POTGMN))
DTT=DT/VOL(I)
C1=DTT*C1
C2=DTT*C2
ST=SO(I)*DL(I)+SG(I)*DG(I)
L=N*(I-1)
DO 20 K=1,N
Z(L+K)=ST*(XL(I)*(X(L+K)-Y(L+K))+Y(L+K))+C1*X(L+K)+C2*Y(L+K)
CONTINUE
CALL SATRN
J=1
DO 30 I=IFRST,ILAST
IF(ICN(J).NE.I) GO TO 32
J=J+1
GO TO 30
32 L=N*(I-1)
ST=SO(I)*DL(I)+SG(I)*DG(I)
DO 31 K=1,N
Z(L+K)=Z(L+K)/ST
CALL FLASH(PNP(I),L,I)
CALL CRTPRP(PNP(I),L,I)
CALL LOOKUP(PCW(I),SG(I),APCO,PPCO,NPCO,IFPCO)
CALL LOOKUP(PCGO(I),SG(I),AFPG,PPCG,NPCG,IFPCG)
CALL LOOKUP(C1,PNP(I),ACO,PCO,NCO,IFCO)
CALL LOOKUP(C2,PNP(I),ACW,PCW,NCW,IFCW)
CALL LOOKUP(C3,PNP(I),ACG,PCG,NCG,IFCG)
B1(I)=CF+SO(I)*C1+SW(I)*C2+SG(I)*C3
CONTINUE
IF(NCOMP.EQ.0) RETURN
WRITE(IO,1006)
FORMAT(10OVERALL COMPOSITION MATRIX*)
DO 51 I=NETA,NCELLS,NETA
WRITE(IO,1007) (NC(J),J=1,5),(Z(N*(I+J-NETA)-9),J=1,NETA)
FORMAT(/,1X,5A2,10F10.6)
DO 51 K=2,N
NA=(K-1)*5
WRITE(IO,1008) (NC(J+NA),J=1,5),(Z(N*(I+J-NETA-1)+K),J=1,NETA)
FORMAT(1X,5A2,10F10.6)
CONTINUE
RETURN
END

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FOOTNOTES

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